ANNUAL REPORT

1998

RESEARCH INSTITUTE FOR SOLID STATE PHYSICS AND OPTICS

of the Hungarian Academy of Sciences, Budapest, Hungary

Research Institute for Solid State Physics
of the Hungarian Academy of Sciences

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ANNUAL REPORT 1998

Edited by **L. Csillag, I. Tüttő, G. Konczos, B. Selmeci**

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Dear Reader,

This booklet summarises the scientific activities of the Research Institute for Solid State Physics and Optics in 1998.

Our Institute was founded by the Hungarian Academy of Sciences in 1981 as part of the Central Research Institute for Physics; in 1992 we became an independent institute with the name : "Research Institute for Solid State Physics".

On the 1st January, 1998 the Crystal Physics Laboratory of the Hungarian Academy of Sciences joined our Institute as a part of the reorganization process of the academic institutes and at the same time the name of the institute has been changed to "Research Institute for Solid State Physics and Optics". In this way our Institute has three new departments: Nonlinear and Quantum Optics, Crystal Physics and Crystal Technology.

The main profile of the Institute is to do basic research in the fields of theoretical and experimental solid state physics and materials science, including metal physics and liquid crystal research, theoretical and experimental optics, including laser physics and the interaction of light with matter. Our experimental research activity is connected to unique methodologies based on large and medium sized facilities like X-ray diffraction, NMR-, Mössbauer-, and optical spectroscopies and neutron scattering experiments at the KFKI Research Reactor.

Some of our research (R & D) activities are more closely related to applications, first of all in the fields of optical thin films, laser applications, crystal growing technologies and metallurgy.

The major part of our research activity is financed by the Hungarian Academy of Sciences and the National Research Fund through supporting individual projects (OTKA). The participation of our research groups in international projects has become more and more significant in supporting our research.

International cooperation plays an important role in the scientific work of our research groups. We have living contacts with a great number of research institutions and universities. In more than half of our publications there are foreign co-authors indicating the significant role of these contacts. The different EU, ESF, COST, NATO and other international projects play a rapidly increasing role in our research activity. It is expected that the share of these resources in our budget will increase with the evolution of the integration process of our country.

Our Institute has been taking part traditionally in gradual and to a larger extent in postgradual education. Details of this activity are also given in this booklet.

An important measure of our results is the number of scientific publications in high quality international journals: we have published more than 170 papers in

international journals and conference proceedings. This number of publications (per scientists) is similar to that in the previous years.

The year 1998 has been a "year of changes" in the life of the Institute, the director has changed too, since the former director Prof. Norbert Kroó undertook a position in the new Hungarian Government.

I hope that this Annual Report gives useful information to the reader. To help to get in contact directly to our scientists, this booklet contains their E-mail addresses too. Our WEB-page may serve further information to the reader.

Budapest, December 1, 1998

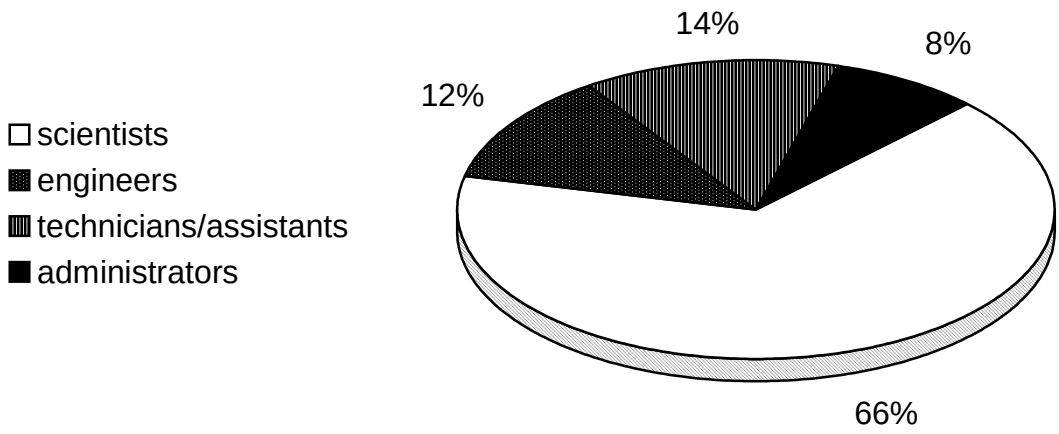
János Kollár

Director

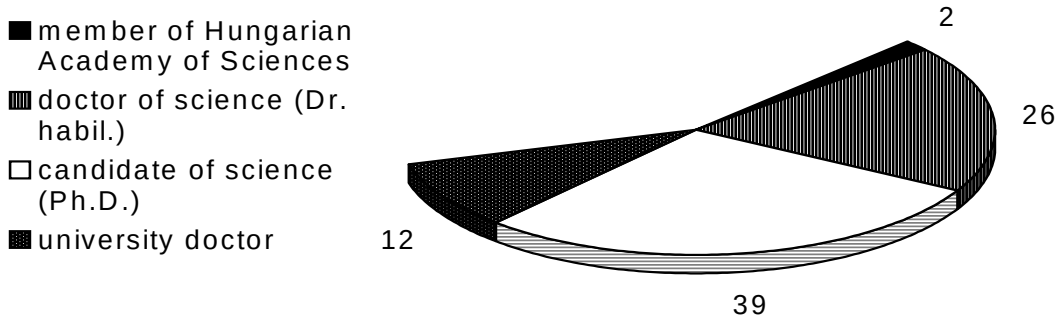
Key figures

Permanent staff of the Institute: 154 employees. Its distribution:

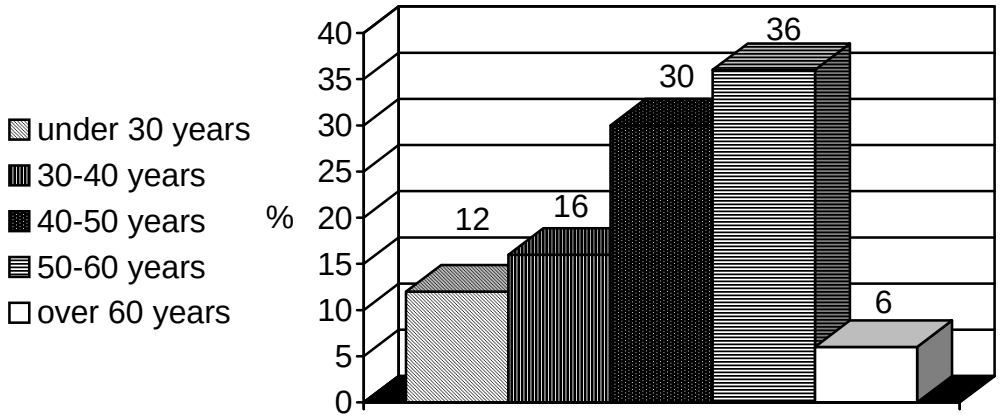
a) by professions:



b) by scientific titles/degrees:

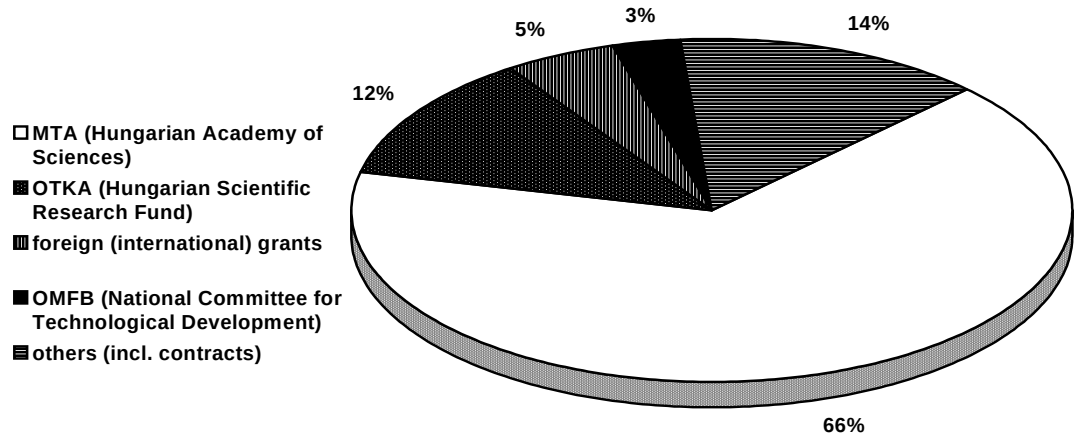


c) by ages:

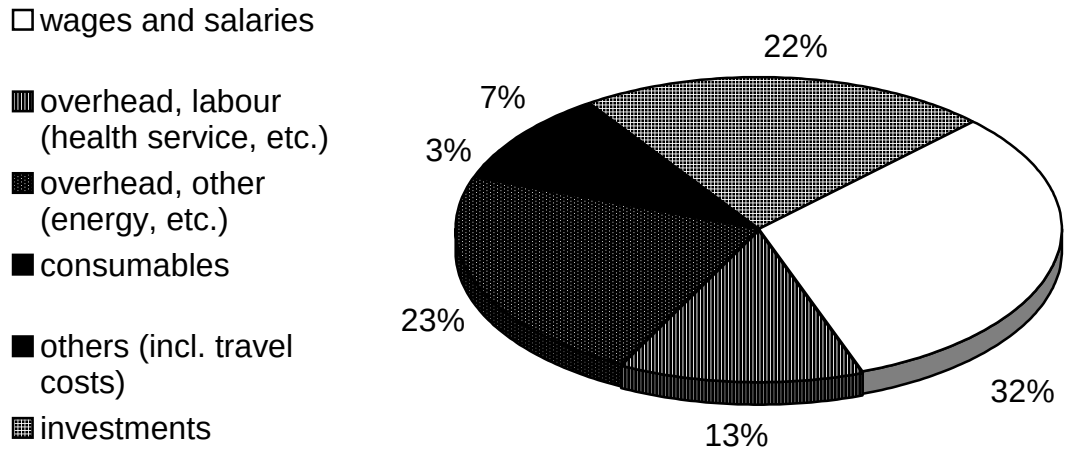


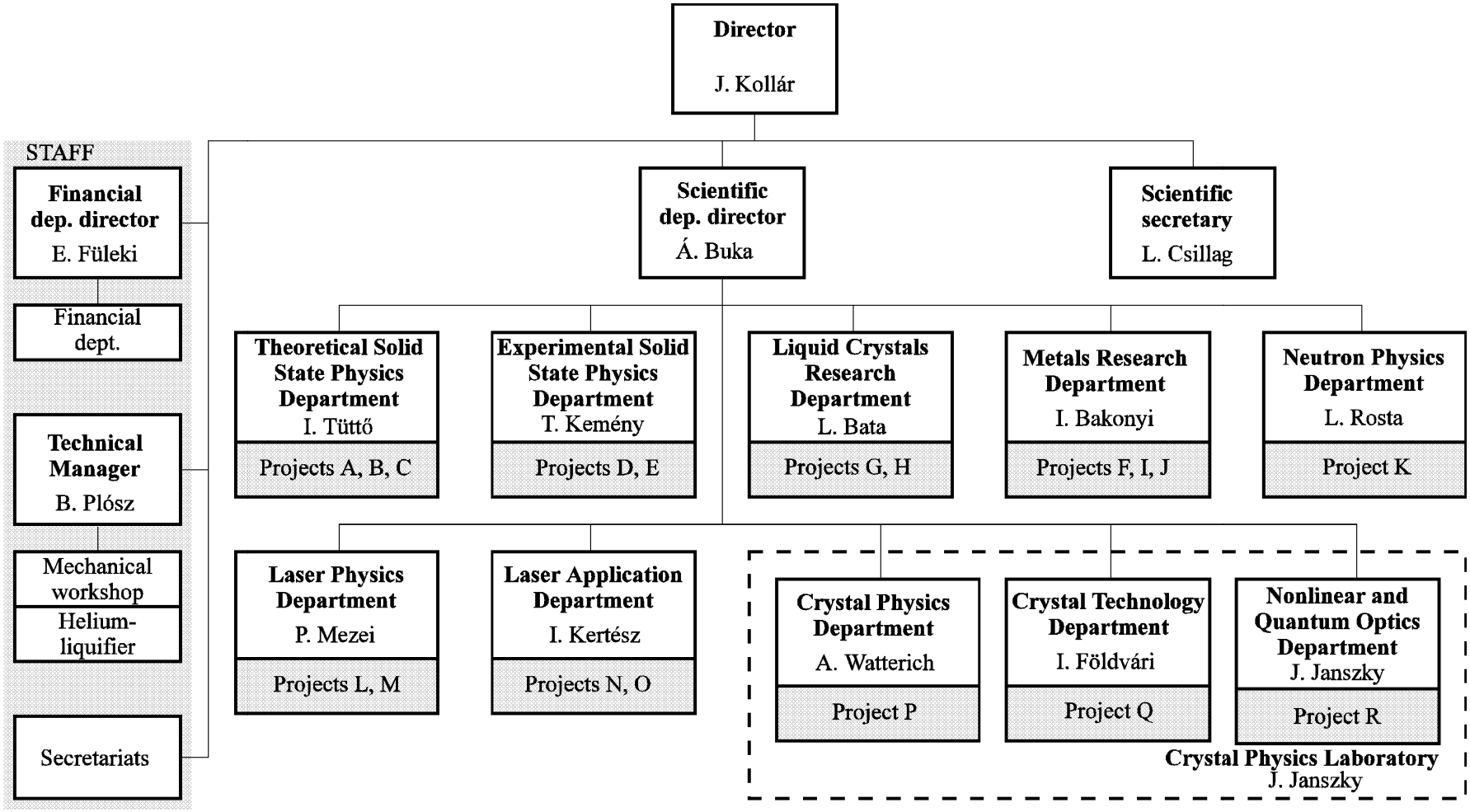
Financial management

a) Sources of operation costs:



b) Distribution of expenditures:





Structure of the Research Institute for Solid State Physics and Optics

A. STRONGLY CORRELATED SYSTEMS

J. Sólyom, G. Fáth, Ö. Legeza, K. Penc, A. Rákos, K. Vladár, F. Woynarovich, A. Zawadowski[+]

Low dimensional magnetic models. — We considered the properties of finite isotropic antiferromagnetic Heisenberg chains with S=1/2, 1, 3/2 spins, when a weak magnetic field is applied on a few sites. It was shown that except for the S=1/2 case uncompensated spins appear at the ends of the chain. The decay of this magnetization has the same character as the decay around the perturbed sites. For the critical, half-odd-integer spin models the exponent of this decay was found to be 1/2, while the exponent of the spin-spin correlation function is η=1. We also analysed the behavior of Haldane-gap antiferromagnets in the opposite limit, in strong magnetic fields. While the low-energy physics of the conventional 1D spin-1 Heisenberg model in its magnetized regime is described by one incommensurate soft mode, other systems with somewhat perturbed coupling constants can possess two characteristic soft modes in a certain range of the field strength. Such a two-component Luttinger liquid phase is realised above the massive Haldane-gap phase, and in general, above any massive nonmagnetic phase, when the ground state exhibits short range incommensurate fluctuations already in the absence of the field.

Most of these calculations used the density matrix renormalization group (DMRG) method. The accuracy of the method depends strongly on the spectrum of the density matrix. For special integrable quantum spin chain models this spectrum can be obtained analytically via the corner transfer matrices (CTM). We have studied in detail the corresponding formulae of the CTM and the reduced density matrix ρ of the DMRG for the transverse Ising chain and the uniaxial XXZ Heisenberg model. Although these systems are integrable and their ground states are known, a direct determination of the corresponding ρ is difficult. We have found that the spectra obtained from DMRG calculation agree well with the CTM results, both in their exponential form and in their predicted degeneracies. Deviations occur only at the lower end where finite-size and geometry effects are visible. In this way we obtained a simple and consistent picture of the density-matrix spectrum and its origin.

We continued studying the scaling limit of the one dimensional XXZ Heisenberg chain. It was found, that the limiting model (obtained in two copies) possesses spin 1/2 massive particles having SU(2) symmetry, and can be identified with the massive sector of the chiral Gross-Neveu model (what is the Sine-Gordon chain at a special coupling).

One-dimensional fermionic models. — We finished the study of the models defined through the relativistic limit of the Hubbard chain by investigating the scaling limit of the one dimensional attractive Hubbard model at less than half filling. Like in the half filled band case, also this model possesses both massive and massless dressed particles. However, unlike the half filled case, only the massive particles are described by Bethe Ansatz type equations, nevertheless the massless excitations still fit into the framework of a conformal field theory.

Theory of dissipative motion of heavy particles. — We studied the low energy physics of fast tunneling centers in metallic environments. For strong enough

[+] Permanent position: Technical University of Budapest

couplings to the environment these tunneling centers display an orbital Kondo effect and give rise to a non-Fermi-liquid behavior. This latter property is explained by establishing a mapping of the tunneling center model to the multichannel Kondo model via the renormalization group transformation combined with a $1/N_f$ expansion. The case of *M*-state systems, the role of the splittings and the present experimental situation were also discussed.

Other topics. — We also showed that the Schrödinger equation for an interacting spinless electron gas in a nonuniform magnetic field admits an exact solution in Jastrow product form when the fluctuations in the magnetic field track the fluctuations in the scalar potential. For tracking realizations in a two-dimensional electron gas, the degeneracy of the lowest Landau level persists, and the "tracking" solutions span the ground state subspace. In the context of the fractional quantum Hall problem, the Laughlin wave function was shown to be a tracking solution. Tracking solutions for screened Coulomb interactions were also constructed. The resulting wavefunctions were proposed as variational wave functions with potentially lower energy in the case of non-negligible Landau level mixing than the Laughlin function.

Finally, propagation failure (pinning) of traveling waves was studied in a discrete scalar reaction-diffusion equation with a piecewise linear, bistable reaction function. The critical points of the pinning transition, and the wavefront profile at the onset of propagation were calculated exactly. The scaling of the wave speed near the transition, and the leading corrections to the front shape were also determined. We found that the speed vanishes logarithmically close to the critical point, thus the model belongs to a different universality class than the standard Nagumo model, defined with a smooth, polynomial reaction function.

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Grants

OTKA[1] T 014443. Completely integrable 1-d systems (F. Woynarovich, 1994-1997)

OTKA T 015870. Models of strongly correlated low-dimensional electron systems (J. Sólyom, 1995-1998)

OTKA T 017128. Theoretical study of dissipative motion of heavy particles (K. Vladár, 1995-1998)

MAKA[2] JF 555/95-B Unconventional behaviour of low-dimensional magnetic and electric systems (J. Sólyom, 1996-1999)

[1] OTKA = Hungarian Scientific Research Fund

[2] MAKA = US-Hungarian Joint Fund

Publications

Articles

A.1. G. Fáth and P. B. Littlewood[*]: Massless phases of Haldane-gap atiferromagnets in a magnetic field. *Phys. Rev.* B **58**, R1234 (1998).

A.2. Ö. Legeza and J. Sólyom: Stability of the Haldane phase in anisotropic magnetic ladders. *Phys. Rev*. B **56**, 14449-14455 (1997).

A.3. T. Antal[*], Z. Rácz[*], A. Rákos, and G. M. Schütz[*]: Isotropic transverse XY chain with energy and magnetization currents. *Phys. Rev. E* **57**, 5184 (1998).

A.4. G. Zaránd[*] and K. Vladár: Orbital Kondo effect from tunneling impurities. *International Journal of Modern Physics* **11,** 2855-2900 (1997).

A.5. G. Fáth and S. B. Haley[*]: Interacting electrons in magnetic fields: Tracking potentials and Jastrow-product wavefunctions. *Phys. Rev.* B **58**, 1405 (1998).

A.6. G. Fáth: Propagation failure of traveling waves in a discrete bistable medium. *Physica D* **116**, 176 (1998).

A.7. Ö. Legeza and J. Sólyom: Response of finite spin-S Heisenberg chains to local perturbations. *Phys. Rev. B.*, accepted for publication

A.8. I. Peschel[*], M. Kaulke[*], Ö. Legeza: Density matrix spectra for integrable models, *Ann. Phys.*, accepted for publication

A.9. F. Woynarovich and P. Forgács[*]: Scaling limit of the one-dimensional attractive Hubbard model: The non-half-filled band case. *Nucl. Phys. B [FS]* (1998), accepted for publication

Book chapter

A.10. F. Woynarovich: Introduction to the coordinate space Bethe Ansatz and to the treatment of the Bethe Ansatz equations. In: *Lecture Notes for Physics* (vol. 498) eds.: Z. Horváth and L. Palla. Springer (1997), pp. 151-203.

[*] The author is not a member of the Research Institute for Solid State Physics and Optics staff

B. COMPLEX SYSTEMS

N. Menyhárd, F. Iglói, A. Sütõ, P. Szépfalusy[+]

The principal interest of this group is the theoretical investigation of different aspects of equilibrium and non-equilibrium statistical physics and quantum systems.

Phase transitions and critical behavior. — We have explored a new fundamental relation between the statistical properties of anomalous diffusion in a random environment and the critical and off-critical behaviour of random quantum spin chains. Many new exact results are obtained from this correspondence including the space and time correlations of surviving random walks and the distribution of the gaps of the corresponding Focker-Planck operator. In turn we have derived analytically the dynamical exponent of the random transverse-field Ising spin chain in the Griffiths region. We have continued the investigation -via computer simulations- the so called parity conserving phase transition (PC) in one dimension. In the non-equilibrium kinetic Ising models the effect of critical fluctuations at the PC transition on the spin system was found to result

1) that the Glauber-Ising process becomes non-Markovian and
2) that the universality class of the compact directed percolation of the spins changes while the compact nature of the clusters remains.

Damage spreading has also been studied in different one-dimensional cellular automata models.

Quantum systems.

a.) A work has been presented on semiclassical quantization and resonance in spin tunnelling.

b.) The investigation of *gases in magnetic traps with Bose condensate* has been continued. The relevant semiclassical behavior of the elementary excitations has been determined in detail. A dielectric formalism has been worked out for such systems and has been used to calculate tha damping of the excitations. The results are in agreement with experimental findings.

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Grants:

OTKA T023642	Phase transitions in quasi-crystals, aperiodic and disordered systems (F. Iglói, 1997-2000)
OTKA T17493	Theory of random processes and complex structures (P. Szépfalusy, 1995-1998)
OTKA T14855	Phase transitions and spectral problem in quantum systems (A. Sütõ, 1995-1998)

[+] Permanent position: Eötvös Loránd University, Budapest

OTKA T023791 Nonequilibrium phase transitions (N. Menyhárd, 1997-2000)
TÉT-F3/96 Critical behaviour of quasi-crystals, aperiodic and disordered systems (F. Iglói, 1997-1999)

Publications

Articles

B.1. F. Iglói, D. Karevski* and H. Rieger*: Random and aperiodic quantum spin chains: a comparative study. *European Physical Journal* **B1,** 513-517 (1998)

B.2. F. Iglói and H. Rieger*: The random transverse-field Ising spin chains and random walks. *Phys. Rev*. **B57,** 11404-11420 (1998).

B.3. E. Carlon* and F. Iglói: Density profiles, Casimir amplitudes and critical exponents in the two dimensional Potts model: a density matrix renormalization study. *Phys. Rev*. **B57,** 7877-7886 (1998)

B.4. F. Iglói, P. Lajkó*, W. Selke* and F. Szalma*: Boundary critical behaviour of two dimensional random Ising models. *J. Phys*. **A31,** 2801-2814 (1998)

B.5. B. Berche*, P-E. Berche*, F. Iglói and G. Palágyi*: The McCoy-Wu model in the mean-field approximation. *J. Phys*. **A31**, 5193-5202 (1998)

B.6. F. Iglói, D. Karevski* and H. Rieger*: Comparative study of the critical behavior in one-dimensional random and aperiodic environments. *European Physical Journal* **B5,** 513-517 (1998)

B.7. J-C. Anglés d'Auriac* and F. Iglói: Level statistics of multispin-coupling models with first and second order phase transitions. *Phys. Rev*. **E58,** 241-246 (1998)

B.8. F. Iglói and H. Rieger*: Anomalous diffusion in disordered media and random quantum spin chains. *Phys. Rev*. **E58,** 4238-4241 (1998)

B.9. N.Menyhárd and G.Ódor*:Non-Markovian persistence at the parity-conserving point of a one-dimensional non-equilibrium kinetic Ising model. *J. Phys. A: Math. Gen*. **30,** 8515-8521 (1997)

B.10. G. Ódor* and N. Menyhárd: Damage spreading for one-dimensional nonequilibrium models with parity conserving phase transitions. *Phys.Rev*. **E57,** 5168-5177 (1998)

B.11. N. Menyhárd and G. Ódor*: Compact parity-conserving percolation in one-dimension. *J. Phys. A: Math. Gen*. **31,** 6771-6781 (1998)

B.12. M. Fliesser*, A. Csordás*, R.Graham* and P. Szépfalusy: Classical quasi-particle dynamics in trapped Bose condensates. *Phys.Rev*. **A56,** 4879-4889 (1997)

B.13. A. Csordás*, R. Graham* and P. Szépfalusy: Semiclassical wave functions and energy levels of Bose-condensed gases in spherically symmetric traps. *Phys. Rev*. **A56,** 5179-5182 (1997)

B.14. A. Csordás*, R. Graham* and P. Szépfalusy : Quasi particle excitations and dynamic structure functions of trapped Bose-condensates in the WKB-approximation, *Phys. Rev*. **A57,** 4669-4685 (1998)

B.15. Gy. Bene*, P. Szépfalusy: Dielectric formalism and damping of collective modes in trapped Bose-Einstein condensed gases, *Phys. Rev.* **A58,** R3391-3394 (1998)

B.16. J.L. van Hemmen* and A. Sütõ: Semiclassical quantization and resonance in spin tunnelling. *J. Phys. A: Math.Gen*. **31,** 1-15 (1998)

C. ELECTRONIC STATES IN SOLIDS

J. Kollár, P. Fazekas, K. Itai, I. Tüttõ, B. Újfalussy, A. Virosztek[+] *, L. Vitos*

We have prepared a review about our recently developed **full charge density** scheme and published it in the Springer Series Lecture Notes in Physics. Using this technique we have established a database of **surface energies** for low index surfaces of 60 metals in the periodic table. The data may be used as a consistent starting point for models of surface science phenomena. The calculated surface energy anisotropies are compared with other density functional theory results and applied in a determination of the equilibrium shape of nano-crystals. We have used our first-principles database in conjunction with the concept of vicinal surfaces to derive the energies of formation of **mono-atomic steps** and corresponding kinks on close-packed surface facets of *bcc* and *fcc* transition metals. The entries in the database allow for a direct calculation of the energies of a number of important steps. For the remaining steps and for all the kinks the energies of formation have been estimated from pair potential expansions of the entries in the database. Furthermore, using the self-consistent jellium model of metal surfaces we investigated the accuracy of a number of semi-local kinetic-energy functionals. Based on this study, we propose a simple one parameter Pade's approximation which reproduces the exact Kohn-Sham surface kinetic energy over the entire range of metallic densities.

A theoretical model based on the screened KKR (Korringa-Kohn-Rostoker) formalism is developed for studying the exchange interaction of two semi-infinite layers separated by a non-magnetic metallic spacer layer which is either pure metal or binary alloy. A first application of the model for pure Cu spacer layer show excellent agrement with experiments, for (100) and (111) facets. We also developed a numerical implementation of method of stationary phase to perform the necessary Brillouin zone integrations. In the employed asymptotic analysis, the relation of the bulk spacer Fermi surface and the periods and damping of the OEC across the spacer emerged in a natural and transparent way. The first application of the model in the OEC (Oscillatory Exchange Coupling) between two Co layers separated by a Cu spacer layer are quite satisfactory and promising for future applications for either pure metallic or disordered alloy spacers.

A review has been prepared about electronic ordering phenomena in orbitally degenerate systems, as part of the Lecture Notes on Electron Correlation and Magnetism (see particularly the Chapters 3, 5, 8, and 11). Apart from yielding the most promising candidate for a lattice fermion model of ferromagnetism (the degenerate Hubbard model with the inclusion of intraatomic exchange), the consideration of orbital degeneracy offers the possibility of novel ordering phenomena. In d-electron systems, an interplay of orbital and spin (and possibly also charge) order has been shown to lead to the dazzling variety of field-induced phenomena in manganites with colossal magnetoresistance. In f-electron systems, spin and charge degrees of freedom cannot be separated, but we can ask whether the order parameter is dipolar, or quadrupolar. It is a closely related question whether the indirect inter-f-shell interactions are derived from direct exchange (leading to customary RKKY) or hybridization (which can give also higher-order couplings).

[+] Permanent position: Technical University Budapest

In the past year we investigated the effect of doping on the strength of the electron-phonon coupling in **high temperature superconductors**. We concluded that the buckling of the CuO_2 planes in the cuprates as well as the strong electron-phonon coupling of the B_{1g} phonon are both due to the electric field across the planes induced by atoms with different valence above and below. We determined the electron-phonon coupling strength from the Raman spectra of various cuprates, which correlate well with reported sizes of buckling, but appear to anticorrelate with the critical temperatures of the samples. This finding lends further support for the electronic origin of high temperature superconductivity.

The Raman spectra of the high T_c materials in the normal state, in the low infrared energy range was interpreted. We have shown, that the spectra can be described using causality arguments, without any model dependent parameters. The measured spectra can be fitted by one functions, by the energy dependent relaxation rate, without any further adjustable parameters. The obtained relaxation rate is highly linear both in temperature and in frequency. The appearence of the pseudogap state shows up as the change in the slope of this relaxation rate around the energy $300cm^{-1}$.

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Levente Vitos	lv@power.szfki.kfki.hu

Grants

OTKA T16740	Electronic states in complex structures (solids, surfaces and interfaces) (J. Kollár, 1995-1998)
OTKA T020030	Interacting electrons in low dimensions (A. Virosztek, 1996-1999)
OTKA T23390	Ab initio study of the structural stability of solids and surfaces (J. Kollár, 1997-2000)
OTKA T022609	Ab initio studies of magnetic thin films (B. Újfalussy, 1997-2000)
OTKA T025505	Competition of ferromagnetism with other collective phenomena in the lattice models for electrons (P. Fazekas, 1998-2001)
OTKA T019045	Collective excitations in unconventional superconductors (I. Tüttõ, 1996-1999)
TÉT -D52/96	Raman scattering in unconventional superconductors (I. Tüttö, 1997-1999)

ESF Network Program Electronic structure calculations (J. Kollár, 1998-2002)

Publications

Articles

C.1. L. Vitos, J. Kollár and H.L. Skriver*: LDA versus GGA: full charge density study of the atomic volume of the light actinides. *Journal of Alloys and Compounds*, **271-273**, 339-341 (1998)

C.2. L. Vitos, A.V. Ruban*, H.L. Skriver* and J. Kollár: The surface energy of metals. *Surface Science* **411,** 186-202 (1998)

C.3. L. Vitos, H.L. Skriver* and J. Kollár: Kinetic energy functionals studied by surface calculations. *Phys. Rev.* B **57**, 12611-12615 (1998)

C.4. T. P. Devereaux*, A. Virosztek, A. Zawadowski, M. Opel*, P. F. Müller, C. Hoffmann*, R. Philipp*, R. Nemetschek*, R. Hackl*, A. Erb*, E. Walker*, H. Berger* and L. Forró*: Enhanced electron-phonon coupling and its irrelevance to high T_c superconductivity. *Sol. State Commun.* **108,** 407-411 (1998)

C.5. L. Vitos, A.V. Ruban*, H.L. Skriver* and J. Kollár: The energetics of steps on transition metal surfaces. *Phil. Mag.* (1998), accepted for publication

C.6. L. Vitos, H.L. Skriver* and J. Kollár: The formation energy for steps and kinks on cubic transition metal surfaces. *Surface Science*, accepted for publication

C.7. B. Újfalussy, N.N. Lathiotakis*, B.L. Gyõrffy*, J.B. Staunton*: Asymptotic behavior of the oscillatory exchange coupling across alloy spacers: a first principles approach. *Phil. Mag.*, accepted for publication

Book, book chapter

C.8. P. Fazekas: Lecture Notes on electron correlation and magnetism. Series in Modern Condensed Matter Physics, Vol. 5, World Scientific (Singapore), pp. 1-777 (1998)

C.9. J. Kollár L. Vitos and H.L. Skriver*: From ASA towards the full potential. *Lecture Notes in Physics, Springer Series*, accepted for publication

D. NON-EQUILIBRIUM ALLOYS

I. Vincze, J. Balogh, L. Bujdosó, D. Kaptás, T. Kemény, L.F. Kiss, Gy. Mészáros, B. Sas, E. Sváb

SQUID Magnetometer. — With the considerable financial support of the National Commitee for Technological Development (OMFB) a Quantum Design produced MPMS 5 SQUID magnetometer was set up in our laboratory. The magnetometer operates in the 1.8-400 K temperature and in the 0-5 T external magnetic field range permitting magnetization measurements with 10^{-7} emu sensitivity. It enables us to measure the magnetic moment of a 5 mm x 5 mm x 4 nm (40 Å) Fe layer with 1 % accuracy. Besides the studies of various amorphous and nanocrystalline samples described below, several cooperations ranging from the studies of different high T_c materials to the investigation of high spin-low spin transformations were initiated. A part of this work is carried out in the frame of the French-Hungarian Scientific and Technology Project (BALATON F-24/97), which also financed the purchase of an external device control board for the magnetometer.

Amorphous and and granular nanocrystalline systems. — Amorphous $Fe_2(B_{1-y}Zr_y)$ alloys being important as the residual amorphous matrix in nanocrystalline Fe-Zr-B-Cu systems, were prepared by rapid quenching from the melt between $0 \leq y \leq 0.55$. The iron magnetic moment determined by ^{57} Fe Mössbauer spectroscopy and magnetic measurements shows an unexpected initial increase when Zr is substituted for B. This behaviour, together with the uncommon crystallization sequence is attributed to the highly attractive B-Zr interaction.

The magnetic behavior of nanosize ferromagnetic *bcc* granules embedded in an amorphous tissue (i.e., partially crystallized $Fe_{80}Zr_7B_{12}Cu_1$ amorphous alloy) was studied by ^{57}Fe Mössbauer spectroscopy. The results are compared with the bulk counterparts: *bcc*-Fe and amorphous $Fe_2B_{0.625}Zr_{0.375}$. Size dependent enhancement of the Curie point of the nanosize amorphous phase was not observed. At temperatures well above the Curie point of the amorphous phase superparamagnetic relaxation of the *bcc* crystallites is observed opening new possibilities to study the anisotropy energy of nano-size ferromagnetic grains.

A critical overview is given for the hyperfine parameters of iron atoms in the nanocrystalline grain boundaries studied for iron nanocrystallites prepared by different methods: ball-milling of iron powder, partial crystallization of Fe-Zr-B-Cu amorphous ribbons and vacuum evaporation of Fe-B polycrystalline multilayers. Careful analysis of the spectral contribution of the possible impurities and the chemical mixing at interfaces reveals that no specific grain boundary contribution can be separated in the Mössbauer spectra when the grain size is in the 2-10 nm range. The results indicate that excluding chemical effects the hyperfine fields of iron atoms in the grain-boundary are very close to those in the bulk and Mössbauer spectra of different nanocrystalline iron samples can be understood without supposing a nanometer sized region of the grain boundary with very distorted structure

Neutron scattering. — The short-range order of $Be_{40}Zr_{60}$ metallic glass was studied by neutron and X-ray diffraction. Two types of model calculations were used: the force algorithm and the iterative procedure based on the Born-Green equation and molecular dynamics using calculated partial pair potentials. A good agreement with experimental structure data has been achieved. All three partial pair correlation functions and

structure characteristics were obtained. It was concluded that the fraction of Zr atoms around Be atoms is considerably higher than the average atomic fraction of Zr and there must be a number of cavities larger than the atomic sphere of Be.

Dynamic neutron radiography was applied for plant research by visualizing and analysing the transport of heavy elements Gd, Sm, Cd (dissolved in D_2O) in bean leaves. The Gd distributed in the main and lateral vascular systems during the first 60 minutes, then there was a penetration into the intercostal tissues. The Sm was transported from the initial drop in the direction of lateral tissues possibly involving cell walls and intercellular space. As regards Cd movement in the course of 30 minutes, it occurred longitudinally in the main vein.

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Grants

OTKA T 020624	Photon- and electron-spectroscopic study of the interfaces of layer structures (J. Balogh, 1996-1999)
OTKA T 020962	Formation and magnetic properties of granular structures (T. Kemény, 1996-1998)
OTKA I/7 T017129	Metastable systems investigated by neutron scattering (E. Sváb, 1995-1998)
OTKA T 022413	Atomic and magnetic structure of nanosystems and interfaces (I. Vincze, 1997-1999)
BALATON F-24/97	Periodic system in random field (B. Sas, 1998-1999)
OTKA I/7 T017129	Metastable systems investigated by neutron scattering (E. Sváb, 1995-1998)

Publications

Articles

D.1. J. Balogh, L. Bujdosó, D. Kaptás, T. Kemény and. I. Vincze: The role of impurities in the crystallization of ball-milled amorphous alloys. *Materials Science Forum* **269-272**, 63-67 (1998).

D.2. T. Kemény, L. K. Varga, L. F.Kiss, J. Balogh, T. Pusztai, L. Tóth* and I. Vincze: Magnetic properties and local structure of Fe-Zr-B-Cu nanocrystalline alloys. *Materials Science Forum* **269-272**, 419-424 (1998).(see also J.3.)

D.3 L.K. Varga, D. Kaptás and T. Kemény: Soft magnetic nanocrystalline powder obtained by mechanical grinding. *Materials Science Forum* **269-272**, 731-736 (1998) (see also J.9.)

D.4. J. Balogh, Z.E. Horváth*, T. Pusztai, T. Kemény and I. Vincze: Absence of evidences of decomposition of Fe_2B during mechanical grinding. *Phys. Rev*. **B57**, 29-32 (1998).(see also E.8.)

D.5. T. Kemény, J. Balogh, I. Farkas*, D. Kaptás, L.F. Kiss, T. Pusztai, L. Tóth* and I. Vincze: Inter-grain coupling in nanocrystalline soft magnets. *J. Phys.: Condens. Matter* **10**, L221-227 (1998). (see also E.9.)

D.6. I. Vincze, T. Kemény, D. Kaptás, L.F. Kiss, and J. Balogh: Nanostructures, disordered ferromagnetism and spin glasses. *Hyperfine Interactions* **113**, 123-134 (1998).

D.7. A. Böhönyey*, G. Huhn*, L.F. Kiss, A. Lovas , I. Gerõcs*: Effect of metalloid substitution on the reversible structural relaxation of Fe-Ni-B(-P, Si) metallic glasses. *J. Non-Cryst. Solids* **232-234**, 490-496 (1998) (see also J.1.)

D.8. A. Lovas, L.F. Kiss, B. Varga, P. Kamasa, I. Balogh, I. Bakonyi: Survey of magnetic properties during and after amorphous-nanocrystalline transformation. *J. Phys. IV (France)* **8**, Pr2/291-298 (1998) (see also I.4. and J.4.)

D.9. F. Sommer*, T. Tarnóczi, K. Russew*, Á. Cziráki*, L.F. Kiss, L.K. Varga, I. Bakonyi: Preparation, structure and physical properties of Fe-, Co- and Ni-rich melt-quenched ribbons containing Zr or Hf. Part IV: Thermal stability: DSC, TEM and thermomagnetic studies. *Z. Metallkde.* **89**, 256-266 (1998) (see also I.6. and J.6.)

D.10 Gy. Mészáros, L. Almásy, E. Sváb, L. Cser, I. Dézsi*: Neutron diffraction study of frozen $Fe(ClO_4)_2$ solutions. *Materials Science Forum*, **278-281,** 732-737 (1998) (see also K.4.)

D.11. M.I. Mendelev*, S.N. Ishmaev*, F. Hajdu, Gy. Mészáros, E. Sváb: Partial structure correlations in amorphous $Ni_{83}La_{17}$. *J. Non-Cryst. Solids* **240,** 35-42 (1998)

D.12 D. Kaptás, T. Kemény, J. Balogh, L. Bujdosó, L.F. Kiss, T. Pusztai and I. Vincze: Magnetic properties of melt-quenched amorphous $Fe_2(B_{1-y}Zr_y)$ ($0 \le y \le 0.55$). *J. Phys.: Condens. Matter* (accepted for publication).

D.13. M. Balaskó*, F. Kőrösi*, E. Sváb, I. Eördögh*: A novel type epithermic neutron radiography detecting and imaging system. *Nuclear Instr & Methods A,* (accepted for publication)

D.14. F. Kõrösi*, M. Balaskó*, E. Sváb: A distribution pattern of cadmium, gadolinium and samarium in Phaseolus vulgaris plants as assessed by dynamic neutron radiography. *Nuclear Instr & Methods A, (*accepted for publication)

D.15 J. Tóth, L.F. Kiss, E. Tóth-Kádár, A. Dinia*, V. Pierron-Bohnes*, I. Bakonyi: Giant magnetoresistance and magnetic properties of electrodeposited $Ni_{81}Cu_{19}$/Cu multilayers. *J. Magn. Magn. Mater*. (accepted for publication) (see also I.11.)

D.16 T. Kemény, D. Kaptás, J. Balogh, L.F. Kiss, T. Pusztai and I. Vincze: Microscopic study of the magnetic coupling between nanoscale phases in a nanocrystalline soft magnet. J. *Phys.: Condens. Matter* (accepted for publication)

D.17 J. Balogh, T. Kemény, I. Vincze, S. Szabó*, D. Beke* and J. Tóth* : Comment on the "Grain boundary structure and magnetic behavior in nanocrystalline ball-milled iron". *Phys. Rev.* (accepted for publication)

Conference proceedings

D.18. M. Balaskó*, E. Sváb, G. Endrõczi*, A. Péter*, I. Szikra*: Radiography investigations combined with vibration diagnostics and acoustic emission in the development of refrigerators. In: *Proc. 7th European Conference on Non Destructive Testing (ECNDT'98)* (Ed. B. Larsen, Copenhagen) (1998) pp.1088-1093

D.19. M. Balaskó*, E. Sváb, I. Cserháti*: Combined dynamic neutron radiography and thermovision in development of absorption-type aggregators. In: *Proc. 7th European Conference on Non Destructive Testing (ECNDT'98)* (Ed. B. Larsen, Copenhagen) (1998) pp.1564-1570

D.20. K. Lázár*, L.F. Kiss, S. Pronier*, G. Onyestyák* and H.K. Beyer*: Iron nanoparticles in X and Y zeolites prepared by reduction with NaN_3. In: *"Mössbauer Spectroscopy in Materials Science", 7-11 September 1998, Senec, Slovak Republic*, NATO ASI, ed.: M. Miglierini (accepted for publication)

D.21. K. Krezhov*, P. Konstantinov*, E. Sváb, Gy. Mészáros: Neutron diffraction investigation of cationic distribution in $Ni_xCo_{3-x}O_4$ spinels. In: *Proc. 6th European Powder Diffraction Conference, 22-25 August, 1998, Budapest (*accepted for publication)

D.22. S.N. Ishmaev*, Z.V. Lisichkin*, A.V. Puchkov*, V.A. Semenov*, E. Sváb, G.F. Syrykh*: Neutron study of dynamic atomic correlations in amorphous isotopic Ni-B alloys. In: *Proc. 6th European Powder Diffraction Conference*, 22-25 August, 1998, Budapest (accepted for publication)

D.23. M.I. Mendelev*, S.N. Ishmaev*, F. Hajdu, Gy. Mészáros, E. Sváb: Short-range order in Be-Zr metallic glass. In: *Proc. 6th European Powder Diffraction Conference,* 22-25 August, 1998, Budapest (accepted for publication)

D.24. M. Balaskó*, E. Sváb: Characterization of segregation by dynamic neutron radiography. In: *Proc. International School and Symposium on Physics in Materials Science - Modification and Characterization of Materials using Nuclear Methods (ISSPMS'98),* Jaszowiec, Poland, 13-19 September 1998 (invited) (accepted for publication)

Other

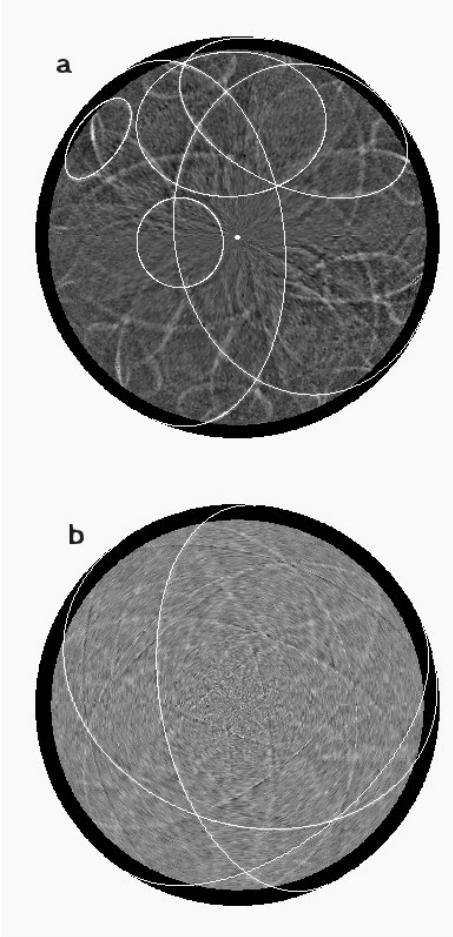
D.25. B. Sas, F. Portier*, I. Puha*, S. Meszaros*, N. Hegman*, K. Vad*, B. Keszei*, F.Williams*: "Pulse measurements of the vortex dynamics". In: *Workshop on*

high Tc superconductors, thin films and applications and vortex dynamics, 27-29 Oct., 1997. Tours, France (in French)

E. X-RAY DIFFRACTION

G. Faigel, G. Bortel, L. Gránásy, K. Kamarás, G. Oszlányi, S. Pekker, T. Pusztai, M. Tegze

Alkali fullerides. — The fullerenes are closed shell molecules containing only carbon atoms. The most abundant among them is the C_{60} molecule. Fullerenes can form a large variety of compounds with elements or other molecules. In the group of A_xC_{60} compounds (A=K,Rb,Cs x=1,3,4,6) there are materials with very interesting properties. Among them many superconducting materials (A_3C_{60}) with remarkably high critical temperature were found. In the last few years the polymeric forms of alkali C_{60} salts became the center of interest. The suggestion of the solid state ionic (2+2) cycloaddition polymerization of singly charged fulleride ions in AC_{60} (A=K, Rb, Cs) salts established a new class of fullerene derivatives. This initiated an extensive study of their structure, of the mechanism of their formation, and of the thermodynamic and the most important physical and chemical properties of these phases. After finding the answers to most of the above questions, we could go further and produce polymers with different bonding configurations and with different dimensionality. We found several stable phases such as Na_2RbC_{60} and Na_4C_{60}. The first one is a singly bonded linear, while the second is a single bonded two dimensional polymer. The stability of these phases was also predicted by our quantum chemical calculations, in which we analyzed the stability of various 1D and 2D polyanions with 1, 2 and 4 sp^3 carbons connected by either (2+2) cycloadduct or by single bonds. We determined the structure and bonding configuration of the Na_4C_{60} from x-ray powder diffraction using Rietveld analysis. This salt has a reversible phase transformation to the monomeric phase at 500 K, and it is the only metal among its A_4C_{60} analogs.

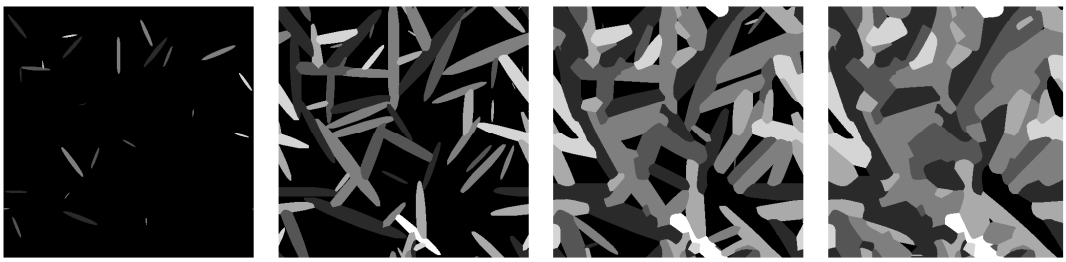


Kossel(a) and standing wave (b) lines of NiO single crystal .

X-ray holography with atomic resolution. — In holography, the scattered radiation is mixed with a reference wave and the resulting interference pattern is recorded. The hologram contains both the intensity and the phase information and the 3 dimensional image of the object can be reconstructed. The most important limitation of this imaging technique is the spatial resolution, which is given by the wavelength and/or by the source size. Using x-rays for hologram forming and the atoms of the sample as sources or detectors atomic resolution can be achieved. We were the first to demonstrate experimentally the feasibility of x-ray holography with atomic resolution on $SrTiO_3$. We also worked on the closely related Kossel lines and standing waves. We have shown that it is possible to detect these patterns using external X-

ray excitation. Further it was demonstrated that structural parameters can be obtained from these patterns (see figure).

Nucleation theory. — We compared the predictions of the latest non-classical theories of crystal nucleation with experiments on stoichiometric oxide glasses (substances for which the most reliable data are available to date). The positive temperature coefficient of the interfacial free energy emerging from experiments is reproduced by only a phenomenological diffuse interface theory we proposed, and by a semiempirical density functional model based on a piecewise parabolic free energy-order parameter relation. It has been demonstrated that the temperature dependence of the interfacial free energy is extremely sensitive to the form of the free energy functional, and that the piecewise parabolic model predicts unphysically broad interfaces (30-50 molecular diameters). This indicates that further work is needed until a fully satisfactory molecular theory of crystal nucleation is developed. Furthermore, we performed a systematic study of the temperature and size dependence of surface tension of the liquid-vapor interface. It has been shown that the Tolman-length, a parameter that describes the size dependence of the surface tension, is positive for small droplets, decreases with increasing size, and tends to a negative value for macroscopic drop, implying that the widely used Tolman-correction is inadequate for typical liquid phase nuclei. We performed Monte Carlo simulations to investigate transformation kinetics during nucleation and anisotropic growth processes (see figure). We have shown that the transformation is slower than predicted by the Johnson-Mehl-Avrami-Kolmogorov model and in the case of pre-existing nuclei it is reasonably described by the mean-field approach of Birnie and Weinberg.



Snapshots of a Monte Carlo simulation for steady state nucleation and random elliptical growth anisotropy.

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Grants

OTKA F020027 X-ray studies of anisotropic and modulated structures (G. Oszlányi, 1997-2000)

OTKA T022041 X-ray holography (M. Tegze, 1997-2000)

OTKA T025139 Theoretical investigation of the dynamics of nucleation and growth processes (L. Gránásy, 1998-2001)

OTKA T016057 Preparation and structural, optical and thermal studies of fullerenes and related materials (G. Faigel, 1995-1998)

OTKA T019139 The study of polymer fullerides and other crystalline C_{60} compounds (S. Pekker, 1996-1999)

AKP 96/2 450 2,2 Structural study of new type of equilibrium and non-equilibrium molecular systems (M. Tegze, 1997-1998)

U.S.-Hungarian Joint Fund 431 Structural study of C_{60} compounds (G. Faigel, 1995-1998)

Publications

Articles

E.1. L. Gránásy, P. F. James*: Nucleation in oxide glasses: comparison of theory and experiment. *Proc. R. Soc. (London) A* **454**, 1745-1766 (1998).

E.2. L. Gránásy, T. Wang*, P. F. James*: Kinetics of wollastonite nucleation in $CaO.SiO_2$ glass. *J. Chem. Phys.***108**, 7317-7326 (1998).

E.3. T. Pusztai, L. Gránásy: Monte Carlo simulations of first-order phase transformations with mutual blocking of anisotropically growing particles up to all relevant orders. *Phys. Rev. B* **57**, 14 110-14 118 (1998).

E.4. G. Oszlányi, G. Baumgartner*, G. Faigel, L. Gránásy, L. Forró*: Polymer-monomer phase transition in Na_4C_{60}. *Phys. Rev. B* **58**, 5-7 (1998).

E.5. S. Pekker, G. Oszlanyi, G. Faigel: Structure and stability of covalently bonded polyfulleride ions in A_xC_{60} salts. *Chem. Phys. Lett.* **282** , 435-441 (1998).

E.6. S. Marchesini*, M. Belakhovsky*, A.Q.R. Baron*, G. Faigel, M.Tegze, P. Kamp*: Standing waves and Kossel line patterns in the structure determination. *Solid State Communication*, **105,** 685-687 (1998)

E.7 T. Gog*, R. A. Eisenhower*, R. -H. Menk*, M. Tegze, G. LeDuc*: Multiple, Energy, X-ray Holography with Atomic Reslolution. *J. Electron Spectr. Rel. Phen.* **92**, 123-129, (1998).

E.8 J. Balogh, Z. E. Horváth*, T. Pusztai, T. Kemény, I. Vincze: Absence of decomposition of Fe_2B during mechanical grinding. *Phys. Rev. B* **57**, 29–32 (1998) (see also D.4.)

E.9 T. Kemény, J. Balogh, I. Farkas*, D. Kaptás, L.F. Kiss, T. Pusztai, L. Tóth*, I. Vincze: Inter-grain coupling in nanocrystalline soft magnets. *J. Phys.: Condensed Matter* **10**, L221–L227 (1998) (see also D.5.)

E.10. K. Kamarás, S. Pekker, L. Forró*, D.B. Tanner*: Infrared and optical spectra of polymerized AC_{60} fullerides. *Chem Phys. Lett.* **295,** 279-284 (1998)

E.11. S.P. Collins*, R.J. Cernik*, B. Fell*, C.C. Tang*, N.W. Harris*, M.C. Miller*, G. Oszlányi: Station 16.3: a high-resolution single-crystal diffraction facility at the SRS Daresbury. *J. Synchrotron Rad.* **5**, 1263-1269 (1998)

E.12. L. Gránásy: Nucleation: free energy of small clusters. Invited for special issue of *Int. J. Non-Equilibrium Processing*, accepted for publication.

E.13. L. Gránásy: Semiempirical van der Waals/Cahn-Hilliard theory: the size dependence of the Tolman-length. *J. Chem. Phys.*, accepted for publication.

E.14. G. Faigel and M. Tegze: X-ray holography, *Report on Progress in Physics*, accepted for publication

E.15. M.C. Miller*, G. Oszlányi, K.S. Ackroyd*, C. Marshall*, S.P. Collins*, D. Laundy*, R.J. Cernik*: PINCER: a portable data-acquisition program based on a command language interpreter, *J. Appl. Cryst.*, accepted for publication

E.16. G. Faigel: Holography with Resonant Quanta, *Hyperfine Interaction*, accepted for publication

E.17. V.C. Long*, J. L. Musfeldt*, K. Kamarás, A. Schilder*, W. Schütz*: Far-infrared study of the Jahn-Teller distorted C_{60} monoanion in C_{60} tetraphenylphosphoniumiodide, *Phys. Rev. B*, accepted for publication.

Conference proceedings

E.18. L. Gránásy, S. Jordery*, I. M. Reaney*, W. E. Lee*, P. F. James*: Crystal nucleation in oxide glasses (invited talk). In: *Proc. of the XVIIIth International Congress on Glass, San Francisco, 1998*, published on CD by The American Ceramic Society.

E.19. S. Pekker, G. Oszlányi, G. Faigel: Total energy calculations of polyfulleride ions. In: *Proc. Conf. on Molecular Nanostructures, Kirchberg,* ed. by H. Kuzmany, J. Fink, M. Mehring and S. Roth, World Sci. Publ. Company 1998, pp. 306-309.

E.20. G. Oszlányi, G. Faigel, G. Baumgartner*, L. Forró*: Two-dimensional polymer structure of Na_4C_{60}. In: *Proc. Conf. on Molecular Nanostructures, Kirchberg,* ed. by H. Kuzmany, J. Fink, M. Mehring and S. Roth, Word Sci. Pub. Company 1998, pp. 343-347.

E.21. K. Kamarás, L. Forró*, Y. Iwasa*, J.L. Musfeldt*: Infrared studies on C_{60} polymers. In: *Proceedings of the 1997 fall Meeting of the Materials Research Society*, Boston, 1998.

Book

E.22 L. Vannay*, A. Tóth*, F. Fülöp*, M. Mezey*, G. Bortel, A. Jákli, L. Gránásy: Fizika laboratóriumi gyakorlatok I – II. (Physics laboratory practices I – II.)

Jegyzet. Budapesti Mûszaki Egyetem, Természet- és Társadalomtudományi Kar, 1998. (in Hungarian) (see also G.19.)

Others

E.23. L. Gránásy: Diffuse interface theory of nucleation: Comparison with experiment and density functional calulations. Abstract Booklet. *72nd ACS Colloid & Surface Science Symposium, June 21-24, 1998, Pennsylvania State University*.

E.24. L. Gránásy, F. Iglói, P. F. James*: Crystal nucleation in liquids and glasses: Comparison of non-classical theories with experiment. Abstract Booklet. *72nd ACS Colloid & Surface Science Symposium, June 21-24, 1998, Pennsylvania State University*.

E.25. G. Faigel: Szinkrotronsugárzás és alkalmazásai (Synchrotron radiation and its applications), *Fizikai Szemle* **48,** 74-77 (1998) (in Hungarian)

F. CHARGE- AND SPIN-DENSITY WAVES

G. Kriza, I. Pethes and G. Mihály[+]

Non-Fermi-liquid behavior in anisotropic metals. — Our understanding of metals lies on the concept of Fermi liquid. In certain anisotropic metals, however, this concept fails fundamentally. A notable example is the quasi-one-dimensional organic conductor $(TMTSF)_2PF_6$. If cooled in a moderate magnetic field of a few teslas, this material undergoes a resistance minimum whereas it remains metallic without magnetic field. We have performed detailed magnetoresistance studies on this compound in order to determine the characteristic magnetic field of the crossover from the metallic to the insulating behavior. We have obtained the highly unexpected result that no such a field exists: the excess resistance due to the magnetic field follows a power law as a function of the strength of the field.

Nuclear magnetic relaxation in charge-density wave systems. — We have studied the nuclear magnetic relaxation in charge-density wave (CDW) systems and showed that the relaxation is dominated by the collective phase excitations of the CDW. We pointed out that the relaxation can be described in a framework common to both charge- and spin-density waves.

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Grants

OTKA TO23786	NMR investigation of collective electronic states in organic conductors (G. Kriza, 1997-2000)
OTKA–NWO (The Netherlands):	Electronic correlations in alkali metal fullerides (A. Jánossy[*], G. Kriza, 1995-1999)

Publications

Articles

F.1 S.E. Brown,[*] W.G. Clark,[*] F. Zámborszky,[*] B. J. Klemme,[*] G. Kriza, B. Alavi,[*] C. Merlic,[*] P. Kuhns,[*] and W. Moulton[*]: ^{13}C NMR measurements of the high-magnetic-field low-temperature phase of $(TMTTF)_2PF_6$. *Phys. Rev. Lett.* **80**, 5429 (1998).

F.2 S.E. Brown,[*] B. Alavi,[*] W.G. Clark,[*] G. Kriza, C. Merlic[*], and F.Zámborszky[*]: High-field NMR studies of $(TMTTF)_2PF_6$. *Synth. Met.* (accepted for publication).

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G. LIQUID CRYSTAL RESEARCH

L. Bata, N. Éber, K. Fodor-Csorba, A. Jákli, E. Szabó, A. Vajda

Study of ferroelectric liquid crystals. — We showed evidences for field induced tilted and horizontally zigzagging layer structures of smectic liquid crystals containing achiral banana-shaped molecules, and gave a qualitative explanation for the observed field-induced-uniform-racemic ground state.

We observed that by suitable electric field treatments the entire smectic film of bent-core molecules can be reversibly transferred to chiral or racemic state. Dielectric, electro-optical and polarization current measurements indicate that the synclinic states have minimum free energies and that the antiferroelectric state is very weak, especially in the chiral state.

Rheology of pyramidic liquid crystals. — We have measured the shear elastic modulus and the viscosity values of a pyramidic liquid crystal both normal and parallel to the columnar axis. The observations can be qualitatively explained by temporary entanglements between the side chains of the bowl-shaped molecules.

Optical alignment of smectic liquid crystals. — It was shown that the light-induced realignment of the director configuration can persist in a nematic-smectic A phase transition and cause rearrangement of the smectic layers within the illuminated area. The ratio between the azimuthal anchoring strengths on the photosensitive and rubbed polyimide plates is estimated.

Silica aggregates in smectic liquid crystals. — Neutron scattering measurements on smectic liquid crystal dispersions containing silica particles with various surface properties indicate that the stability of the memory correlates to the number of OH groups on the silica surfaces. These observations imply that, with fine-tuning of the OH content of the silica surfaces, various types of memory devices can be designed.

Synthesis of liquid crystals. — Deuterium labelled double bond containing chiral liquid crystals have been prepared and investigated, later polymerized giving chiral ferroelectric liquid crystals. Their behaviour was investigated either by X-ray or ^{2}H NMR spectroscopy.

New achiral bent shaped molecules derived from cinnamic acids were also prepared containing more than three benzene rings in their core. Their mesophase behaviour was established by optical microscopy and differential scanning calorimetry.

Some new ferroelectric mixtures have also been investigated. New chiral compounds have been developed either as additives in the above mixtures or for polymerization to have new ferroelectric polymeric liquid crystals.

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Grants:

OTKA T-016252 Study of ferroelectric liquid crystals (Lajos Bata, 1995-1998)
OTKA T-020905 Deuterium labeling of liquid crystals (K. Fodor-Csorba, 1997-2000)
OTKA T-022772 Viscoelastic properties of smectic liquid crystals (Nándor Éber, 1997-2000)
OTKA T-023102 Investigation of physical properties of columnar and cubic mesophase (Antal Jákli, 1997-2000)
TÉT GB-75/96 Synthesis and characterization of novel ferroelectric liquid crystals for display applications (Lajos Bata, 1996-1998)
Volkswagen Foundation (German-Hungarian bilateral): Study of ferroelectric columnar phases (Antal Jákli, 1997-1998)
ERBIC15CT960744 INCO Copernicus EC Research Network: Novel techniques and models for the surface treatment of liquid crystals with optical applications (Antal Jákli, 1997-1999)

Publications

Articles

G.1. L. Almásy, A. Jákli, L. Rosta and G. Pépy*: Structural memory effect in liquid crystal phases stabilised by silica particle aggregates. *Physica B,* **241-243**, 996-998 (1998) (see also K.1.)

G.2. A. Jákli, M. Müller*, D. Krüerke* and G. Heppke*: First observation of electromechanical effects in a chiral ferroelectric columnar liquid crystal. *Liq. Cryst.* **24**, 467-472 (1998)

G.3. A. Jákli, S. Rauch*, D. Lötzsch* and G. Heppke*: Uniform textures of a smectic liquid crystal phase formed by bent-core-molecules. *Phys. Rev. E,* **57**, 6737-6740 (1998)

G.4. K. Fodor-Csorba, A. Jákli, A.Vajda, E. Szabó, L.Bata, G.Galli*, S.Holly*, E.Gács-Baitz*, L.C.Chien*: Synthesis and properties of chiral liquid crystalline terephthalic acid derivatives. *Liquid Crystals* **24**, 861-869 (1998)

G.5. A. Jákli: Electromechanical responses of antiferroelectric and ferrielectric liquid crystals. *J. Appl. Phys.*, accepted for publication

G.6. M. Giocondo*, A. Jákli, A. Saupe*: Tilted smectic layers of a smectic liquid crystal between homeotropically treated plates. *The European Physical Journal B.*, accepted for publication

G.7. T. Tóth Katona, N. Éber, Á. Buka: Thermally induced ageing in bicyclohexyl compounds and its influence on the N-SmB phase transition and interface morphology. *Mol.Cryst.Liq.Cryst.*, accepted for publication (see also H.10.).

G.8. G. Pelzl*, S. Diele*, A. Jákli, Ch. Lischka*, I. Wirth*, W. Weissflog*: Helical superstructures in a novel smectic mesophase formed by achiral banana-shaped molecules. *Liquid Crystals* (1998), accepted for publication

G.9. G. Pelzl*, S. Diele*, S. Grande*, A. Jákli, Ch. Lischka*, H. Kresse*, H. Schalmfuss*, I. Wirth*, W. Weissflog*: Structural and electro-optical investigations of the smectic phase of a chlorine-substituted banana-shaped compounds. *Liquid Crystals* (1998), accepted for publication

Conference proceedings

G.10. A. Jákli: Piezoelectricity and ferroelectricity of columnar liquid crystals. In: *Proc. of 4th Indian National Seminar on Liquid Crystals, Patiala, India,* Printed in Bangalore, (1998), pp. 1-8.

G.11. A. Vajda, J. Hajtó*, J. Wright*, K. Fodor-Csorba, I. Jánossy, L. Bata, G. H. W. Milburn*: Ferroelectric mixtures containing fluorine derivatives. In: *Proceedings of ECLC'97, Zakopane, Poland,* Eds. J. Rutkowska, S. J. Klosowicz, J. Zielinski and J. Zmija, *SPIE,* **3318,** 82-85. (1998) (see also H.12.)

G.12. J. Gruber*, M. C. Schraber*, J. Hajtó*, A. Vajda, K. Fodor-Csorba, I. Jánossy: Dielectric and electrooptic studies of a novel ferroelectric mixture. In: *Proceedings of ECLC'97, Zakopane, Poland,* Eds. J. Rutkowska, S. J. Klosowicz, J. Zielinski and J. Zmija, *SPIE,* **3318**, 78-81(1998). (see also H.11.)

G.13. K. Fodor-Csorba*, T. Paksi, A. Vajda, S. Holly*, E. Gács-Baitz*, A. Dobó*, A. Jákli: Chemical processes in liquid crystal composite systems containing cholesteryl propionate. In: *Proceedings of ECLC'97, Zakopane, Poland,* Eds. M. Tykarska, R.Dabrowski and J. Zielinski, *SPIE,* **3319,** 191-194 (1998).

G.14. D. Z. Obadovic*, M. Stancic*, L. Bata, A. Vajda: Study of the influence of ionizing radiation onto phase transitions of mixtures of some cholesteric liquid crystals. In: *Proceedings of ECLC'97, Zakopane, Poland,* Eds. M. Tykarska, R.Dabrowski and J. Zielinski, *SPIE,* **3319,** 195-197 (1998).

G.15. D. Z. Obadovic*, A. Vajda, S. Jovanovic-Santa*, M. Stancic*, J. Petrovic*: The influence of new chiral additives on phase transitions of binary mixtures of some cholesteric liquid crystals. In: *Proc. of 6th European Powder Diffraction Conference, Budapest, Hungary,* Eds. R. Delhez and E. J. Mittemeijer, *Mat. Sci. Forum* (Trans. Tech. Publications, Switzerland), accepted for publication

G.16. D. Z. Obadovic*, A. Vajda, M. Stancic*, D. Lazar*, K. Fodor-Csorba, L. Bata: The study of phase transitions of binary liquid crystalline mixtures. In: *Proc. of 6th European Powder Diffraction Conference, Budapest, Hungary,* Eds. R. Delhez and E. J. Mittemeijer, *Mat. Sci. Forum* (Trans. Tech. Publications, Switzerland), accepted for publication

Books, book chapters

G.17. A. Jákli: Electrically induced vibrations and flows in ferroelectric liquid crystals. In: *Dynamics and defects in liquid crystals* Ed.: P. Cladis and P. Palffy-Muhoray, Gordon & Breach (1998), pp. 321-329.

G.18. K. Fodor-Csorba: Pesticides in environmental samples. In *Advanced Chromatographic and Electromigration Methods in Biosciences*. Eds. Z. Deyl,

I. Miksik, F. Tagliaro, E. Terasova, J. of Chromatography Library, Elsevier, Amsterdam, **60,** 779-831 (1998).

G.19 L. Vannay*, A. Tóth*, F. Fülöp*, M. Mezey*, G. Bortel, A. Jákli, L. Gránásy: Fizika laboratóriumi gyakorlatok I – II. (Physics laboratory practices I – II.) Jegyzet. Budapesti Mûszaki Egyetem, Természet- és Társadalomtudományi Kar, 1998. (in Hungarian) (see also E.22.)

Others

G.20. A. Jákli: Making perfect chiral smectic C displays and rehealing them by guided backflow. *LCI Online Electronic Journal*, June 1998. http:\\www.lcionline.net

G.21. K. Fodor-Csorba, L. Bata, S. Holly*, E. Gács-Baitz*: Stabil izotóppal jelzett termotróp folyadékkristályok előállítása és vizsgálata I. (Synthesis and investigation of thermotropic liquid crystals labelled by stable isotopes I., in Hungarian) *Magyar Kémiai Folyóirat* **104**, 349-353 (1998).

G.22. V. Vargha*, K. Fodor-Csorba, A. Pozsgay*: Ferroelektromos folyadékkristály polimerek (Ferroelectric polymeric liquid crystals, in Hungarian). *Mûanyag és Gumi* **35**, 11-17 (1998)

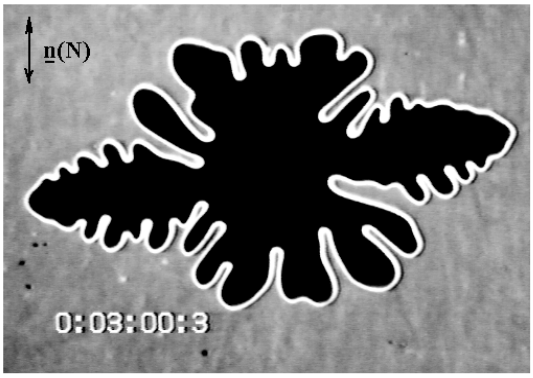
H. INSTABILITIES AND NONLINEAR PHENOMENA IN LIQUID CRYSTALS

Á. Buka, T. Börzsönyi, D. Goldschmidt, I. Jánossy, T. Tóth-Katona

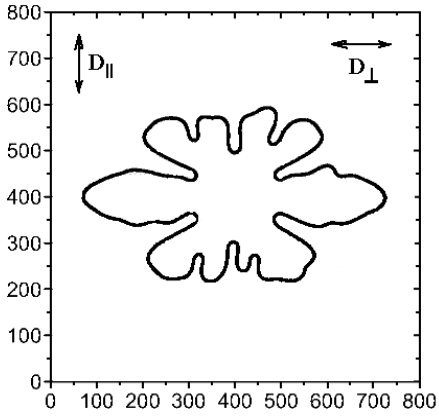
Pattern formation:

– *Oscillatory shear induced instabilities.* — The precession of the director was generated by elliptic shear and high frequency oscillatory compression in a homeotropic nematic liquid crystal layer in the presence of a destabilizing electric field. The precession frequency was found orders of magnitude smaller than that of the external driving shear. Its dependence on the amplitude and frequency of the shear is in accordance with the predictions of the linear calculations. The voltage dependence is non-monotonous, and needs a more complex description. The spatiotemporal behavior of the system leads to the formation of spiral patterns.

– *Nematic - smectic B interface.* — Experiments and numerical simulations concerning the influence of the heat diffusion anisotropy have been extended to a new geometry (homeotropic smectic B in planar nematic). In this system the surface tension anisotropy is much smaller than in case of planar alignment of both phases. The surface tension and kinetic anisotropies have been estimated by numerical simulations based on the phase-field model. Besides the experimental and numerical methods it has been shown analytically that a crystal in an environment with anisotropic heat diffusion coefficient grows faster in the direction of the low heat diffusion ($D_\perp < D_{||}$, see figures).



experiment



simulation

An experimental evidence has been given that thermally induced aging, observed in investigated substances is caused by the air atmosphere, and its effect on the pattern formation has been described.

– *Viscous fingering.* — In a radial Hele-Shaw cell geometry, the influence of the effective viscosity (tuned by an applied electric field) on the morphology and dynamics of the nematic - air interface has been mapped as a function of the excess pressure.

– *Electrohydrodynamic instabilities.* — Experiments have been carried out in nematics with homeotropic alignment where the electrohydrodynamic instability occurs after a bend Freedericksz transition. The threshold of the convection, the wave number at onset, and the threshold for the transition between order and disorder in the presence of a stabilizing magnetic field agree with theory. Whereas

in the oblique-roll range the behavior of the correlation time of the disordered state in the normall-roll range at zero magnetic field shows no dynamics below well defined value ε_s of the reduced control parameter, in contrast to theoretical predictions. At ε_s one has reproducibly a continuous and reversible transition to a dynamic state. We attribute these features to the appearance of chevronlike structures.

Non-linear optics:

– *Laser-induced effects in liquid crystals.* — The enhancement of light induced reorientation was studied in the presence of dyes, showing trans-cis isomerization. The enhancement factors of the trans and cis forms were determined separately; the former isomer exhibited a large negative, while the latter one a large positive factor. This behaviour was related to the changes of the shape of the dye molecules during trans-cis transitions.

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Grants:

OTKA T-014957 Structure formation in non equilibrium, complex systems (Ágnes Buka, 1995-1998)
OTKA T-024098 Laser induced phenomena in smectic liquid crystals (István Jánossy, 1997-2000)
OTKA F-022771 Interfacial patterns and convective instabilities (Tibor Tóth-Katona, 1997-2000)
Volkswagen Foundation (German-Hungarian bilateral) Pattern formation in liquid crystals (Ágnes Buka, 1997-1998)
ERB FMRX-CT 96-0085 EC Research Network: Pattern formation, noise and spatio-temporal chaos (Ágnes Buka, 1996-2000)

Publications

Articles

H.1. R. González-Cinca*, L. Ramírez-Piscina*, J. Casademunt*, A. Hernández-Machado*, T. Tóth-Katona, T. Börzsönyi and Á. Buka: Heat diffusion anisotropy in dendritic growth: phase field simulations and experiments in liquid crystals. *J. Cryst. Growth,* **193,** 712-719 (1998)

H.2. P. Tóth* , Á. Buka, J. Peinke* and L. Kramer*: Dynamics of disordered patterns in electroconvection of homeotropically aligned nematic liquid crystals. *Phys. Rev.* **E58,** 1983-1991 (1998)

H.3. I. Jánossy and L. Szabados: Optical reorientation of nematic liquid crystals in the presence of photoisomerization. *Phys. Rev.* **E58**, 4598-4604 (1998)

H.4. T. Börzsönyi, Á. Buka and L. Kramer*: Effect of the anisotropic surface tension, crystallization kinetics, and heat diffusion in nonequilibrium growth of liquid crystals. *Phys. Rev.* **E58,** 6236-6245 (1998)

H.5. L. Szabados, I. Jánossy and T. Kósa: Laser-induced bulk effects in nematic liquid crystals doped with azo dyes. *Mol. Cryst. Liq. Cryst.*, **320**, 239-248 (1998)

H.6. D.M. Goldschmidt, V.S. Zykov* and S.C. Müller*: Transition to irregular dynamics of spiral waves under two-channel feedback. *Phys. Rev. Lett.*, **80**, 5220-5223 (1998)

H.7. I. Jánossy and L. Szabados: Photoisomerization of azo dyes in nematic liquid crystals. *Journ. Nonlinear Opt. Phys. Mater.* **7**, No. 4 (1998)

H.8. T. Börzsönyi, Á. Buka, A.P. Krekhov* and L. Kramer*: Response of a homeotropic nematic liquid crystal to rectilinear shear. *Phys. Rev. E,* accepted for publication

H.9. S. Thiberge*, C. Chevallard*, Á. Buka and J.M.Gilli*: Critical radius of loop defects in a homeotropic nematic liquid crystal. *Liq. Cryst.*, accepted for publication (Preprint INLN, Nice, No.97.36)

H.10. T. Tóth-Katona, N. Éber and Á. Buka: Thermally induced ageing in bicyclohexyl compounds and its influence on the N – SmB phase transition and interface morphology. *Mol. Cryst. Liq. Cryst.*, accepted for publication (see also G.7.)

Conference proceedings

H.11. J. Gruber*, M.C. Schraber*, J. Hajtó*, A. Vajda, K. Fodor-Csorba and I. Jánossy: Dielectric and electrooptic studies of a novel ferroelectric liquid crystal mixture. In: *Proceedings of ECLC'97, Zakopane, Poland,* Eds. J. Rutkowska, S.J. Klosowicz, J. Zielinski and J. Zmija, *SPIE* **3318,** 78-81 (1998) (see also G.12.)

H.12. A. Vajda, J. Hajtó*, J. Wright*, K. Fodor-Csorba, I. Jánossy, L. Bata and G.H.W. Milburn*: Ferroelectric mixtures containing fluorine derivatives. In: *Proceedings of ECLC'97, Zakopane, Poland,* Eds. J. Rutkowska, S.J. Klosowicz, J. Zielinski and J. Zmija, *SPIE* **3318,** 82-85 (1998) (see also G.11.)

H.13. T. Börzsönyi, A.P. Krekhov*, O.A. Scaldin and Á. Buka: Pattern formation in a homeotropic liquid crystal induced by rectilinear and elliptical shear. In: *Proceedings of ECLC'97, Zakopane, Poland*, Eds. M. Tykarska, R. Dabrowski and J. Zielinski, *SPIE* **3319,** 129-132 (1998)

Book

H.14. D.Ž. Obadović*, M. Stančić* and T. Tóth-Katona: Fizika Tečnih Kristala sa Primenama (Physics of Liquid Crystals with Applications, in Serbian).

University of Novi Sad, Faculty of Natural Sciences and Mathematics, Novi Sad (1998)

I. METAL PHYSICS

K. Tompa, I. Bakonyi, M. Bokor[+] *, J. Garaguly, Cs. Hargitai, Gy. Lasanda, T. Marek*[++] *, L. Péter, J. Tóth, E. Tóth-Kádár*

Metal-hydrogen systems. — In the study of amorphous alloy-hydrogen systems low temperature ("rigid lattice") ^{1}H NMR spectrum shape and second moment (M_2) have been measured in $\mathbf{Zr}_y\mathbf{(Ni}_{1-x}\mathbf{Cu}_x\mathbf{)}_{1-y}\mathbf{-H}$ ternary amorphous alloys of different hydrogen content at $0 \leq x \leq 33$ at % **Cu** and y = 33, 50 and 67 at % **Zr** concentrations using FID and solid-echo pulse sequences. The line shape can be described by the Harper-Barnes function with continuously changing exponent in the function of the hydrogen content. The second moment-hydrogen concentration data (as seen in the figure below) can be fitted by a power function of 3/4 exponent. The interpretation shows an inhomogeneous hydrogen distribution and local fields originating from a few proton neighbours.

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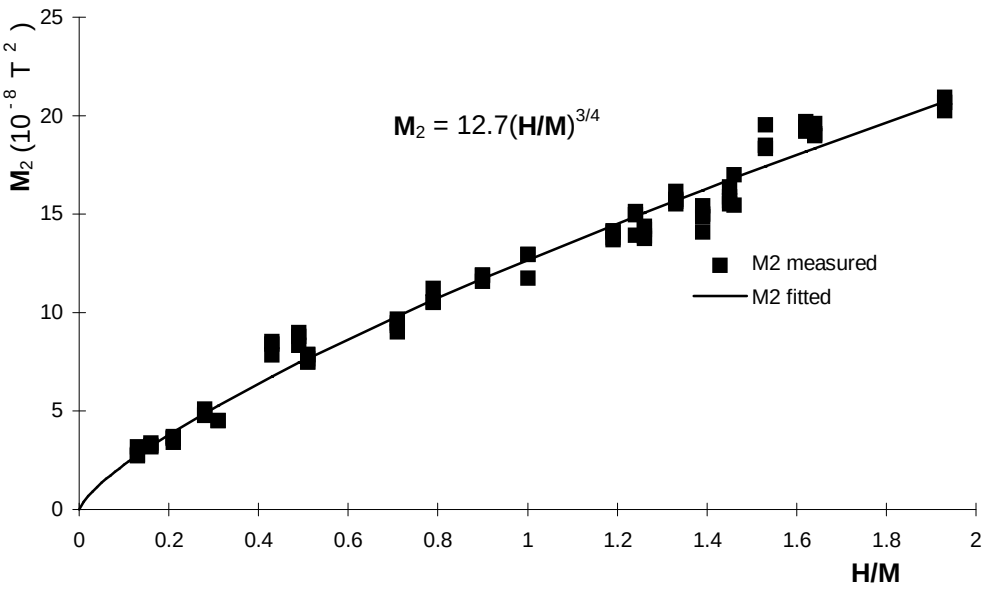

The carefully measured amplitude of the *CPMG* echo-train, the gas-chromatographic and prompt gamma activation analysis data of the same system give different values for the hydrogen content in the "motional narrowing" state, demonstrating the partition of hydrogen in disordered systems, proving that not all the hydrogen take part in the diffusion process.

In-situ-NMR, electrical resistivity and positron annihilation measurement were started on $\mathbf{Pd}_{0.8}\mathbf{Ag}_{0.2}\mathbf{-H}$ crystalline alloy, on a model material representing a chemically disordered system for the hydrogen storage. The in-situ NMR measurements realised first in the world in a hydrogen storing metal gives unique chance for the investigation of hydrogen charging, discharging and diffusion processes.

[+] *Ph.D. student (Eötvös University) supported also by the HAS and the Soros Foundation Hungary*

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Transition metal complexes. — Continuing the study of transition metal complexes ^{19}F and ^{11}B NMR spectra and spin-lattice relaxation times were measured and interpreted in $[Zn(ptz)_6](BF_4)_2$ (ptz = 1-*n*-propyl-1H-tetrazole) and in $[Fe(ptz)_6](BF_4)_2$ between room temperature and 2.2 K. The characteristics of the molecular motions of the BF_4 ion and CH_3 group were evaluated . Similarly to the proton NMR results, clear signs of presence of high-spin state Fe^{2+} ions at low temperatures were detected in ^{19}F and ^{11}B NMR parameters. Additionally, static magnetization measurements were done in the whole temperature range, and the low temperature results, contrary to the high temperature ones can not be described by a Brillouin function.

Metastable metallic phases. — Recently, we have reported that, for the first time, a single-phase, fully nanocrystalline alloy could be produced directly from the melt: for a sufficiently high cooling rate, the melt-quenching of a $Hf_{11}Ni_{89}$ alloy resulted in a nanocrystalline $HfNi_5$ structure without any detectable other phases. In exploring the factors governing nanocrystalline-forming ability (NFA), we should look for alloy compositions where we can expect a high rate of homogenous nucleation. Evidently, this should occur at stoichiometric compositions. The stoichiometric composition ensures that the compound formation can occur without the necessity of a phase separation, i.e., long-range atomic rearrangements in the melt and, therefore, it can proceed homogeneously throughout the whole volume. Obviously, the more stable is the compound, the stronger is the driving force for its formation while cooling the melt. Accordingly, the applied cooling rate should remain below the critical cooling rate for amorphous phase formation (r_{ca}) but still sufficiently high to prevent grain growth in order to retain the nanocrystalline state. For a given alloy composition, this lower critical cooling rate is denoted as r_{cn} where the subscript *n* refers now to the formation of nanocrystalline state. By considering a stoichiometric composition and a homogeneous nucleation of the compound crystallites from the melt, the grain growth is governed by atomic diffusion. In alloys composed of atoms with significantly different diameters, the diffusion of one component may be strongly hindered and this fact may effectively block further grain growth of the developed nanocrystalline state. In such cases, the application of cooling rates in the range $r_{cn} < r < r_{ca}$ may strongly promote the formation of a nanocrystalline state. Exceeding the critical cooling rate r_{cn} is necessary in this scheme in order to effectively prevent grain growth by not allowing sufficient time for atomic diffusion. According to the discussions above, prospective candidates exhibiting high NFA by melt-quenching can be alloy compositions of stoichiometric compounds formed by elements of differring atomic radii. This new way of producing nanocrystalline alloys directly from the melt

(i) opens up the possibility of preparing nanocrystalline alloys at previously unaccessible compositions;

(ii) can yield large quantities of bulk, porosity-free nanocrystalline alloys;

(iii) will facilitate the interpretation of results on various physical properties of nanocrystalline alloys since this technique could make available samples with a single phase present.

Metallic multilayers — Electrodeposited Ni-Cu alloys and nanoscale $Ni_{81}Cu_{19}$/Cu multilayers were produced by direct-current plating and pulse-plating, respectively. The room-temperature electrical resistivity and thermopower were investigated for the Ni-Cu electrodeposits as a function of composition and for the $Ni_{81}Cu_{19}$/Cu multilayers as a function of the constituent magnetic and non-magnetic layer

thicknesses. For the multilayers, the calculated resistivity values obtained in a parallel resisitance model based on bulk resistivities of the sublayer materials remained significantly below the experimental data although they approached towards them with increasing sublayer thicknesses. The main origin of the observed discrepancy lies in the nanoscale multilayer structure. Namely, it has been well documented in the literature that in thin films of similar thicknesses as the sublayers in our multilayers, a significant surface scattering of electrons can greatly enhance the electrical resistivity beyond the bulk values and the same should happen also at the interfaces in the multilayer structure. The importance of these effects is exemplified by the fact that for multilayer series with a constant Cu thickness of about 1 nm, the experimental resisitivity data exceeded the parallel resistance model by about a factor of two even for d_{Ni-Cu} as high as 10 nm. The experimental thermopower data were found to be more negative than by simply taking a volume average of the bulk values of the constituent sublayers. An increased surface scattering effect might be responsible also here for the difference although it is hard to make even a qualitative estimate at present to take into account the influence of surface scattering on thermopower of nanoscale multilayer films. On the other hand, the present study indicated a diffrence in sensitivity of the electrical resistivity and the thermopower to surface scattering processes as manifested also in the relatively good agreement of calculated and measured thermopower values for magnetic layer thicknesses where the parallel resistance model was still well below the experimental data.

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Grants

OTKA T015649	Giant magnetotransport phenomena in nanophase metals (I. Bakonyi, 1995-1998)
OTKA T016670	NMR relaxation and local properties in solids (K. Tompa, 1995-1998)
OTKA T 022 124	Preparation and investigation of single-phase nanocrystalline metals (I. Bakonyi, 1997-2000)
AKP 97-48 2,2/37	Hydrogen diffusion and chemical order in hydrogen storing Pd-Ag alloys, K. Tompa, 1998-1999)

Publications

Articles

I.1. M. Bokor, T. Marek*, K. Süvegh*, K. Tompa, A. Vértes*: Fe^{2+} spin-crossover complexes: structure and positron annihilation. *Mater. Sci. Forum* **255-257**, 281-283 (1997)

I.2. Á. Cziráki*, I. Gerõcs*, B. Fogarassy*, G. Van Tendeloo*, F. Sommer*, I. Bakonyi: Study of the thermal decomposition of melt-quenched Ni-rich metastable bcc and amorphous Ni-Zr alloys. *Int. J. Non-Equilibr. Proc.* **10**, 265-282 (1998)

I.3. Á. Cziráki*, V. Pierron-Bohnes*, C. Ulhaq-Bouillet*, E. Tóth-Kádár, I. Bakonyi: A cross-sectional high-resolution transmission electron microscopy study of electrodeposited Ni-Cu/Cu multilayers. *Thin Solid Films* **318**, 239-242 (1998)

I.4. A. Lovas, L.F. Kiss, B. Varga, P. Kamasa, I. Balogh, I. Bakonyi: Survey of magnetic properties during and after amorphous-nanocrystalline transformation. *J. Phys. IV (France)* **8**, Pr2/291-298 (1998) (see also D.8. and J.4.)

I.5. L. Pogány, D.T. Son*, I. Varga, Z. Fülöp*, C. Hargitai, I. Bakonyi: Measurement of internal magnetic domain structures by using backscattered electrons in a SEM. *J. Phys. IV (France)* **8**, Pr2/697-700 (1998) (see also J.5.)

I.6. F. Sommer*, T. Tarnóczi, K. Russew*, Á. Cziráki*, L.F. Kiss, L.K. Varga, I. Bakonyi: Preparation, structure and physical properties of Fe-, Co- and Ni-rich melt-quenched ribbons containing Zr or Hf. Part IV: Thermal stability: DSC, TEM and thermomagnetic studies. *Z. Metallkde.* **89**, 256-266 (1998) (see also D.9. and J.6.)

I.7. I. Bakonyi, Á. Cziráki*: Nanocrystalline-forming ability of alloys by melt-quenching. *Nanostruct. Mater.*, accepted for publication

I.8. I. Bakonyi, E. Tóth-Kádár, J. Tóth, L. Pogány, T. Tarnóczi, P. Kamasa: Magnetic and electrical transport properties of electrodeposited Ni-Cu alloys and $Ni_{81}Cu_{19}$/Cu multilayers. *J. Phys. Cond. Matter*, accepted for publication (see also J.12.)

I.9. Á. Cziráki*, J.G. Zheng*, A. Michel*, Zs. Czigány*, G. Nabiyouni*, W. Schwarzacher*, E. Tóth-Kádár, I. Bakonyi: Cross-sectional high-resolution transmission electron microscopy study of the influence of preparation conditions on the microstructure of electrodeposited Co-Ni-Cu/Cu multilayers. *Z. Metallkde.*, accepted for publication

I.10. R. Lück*, Z.F. Dong*, M. Schieffer*, I. Bakonyi, K. Lu*: Mictrostructure identification of an interfacial phase in a melt-spun Hf-Ni nanocrystalline alloy. *Phil. Mag.*, accepted for publication

I.11. J. Tóth, L.F. Kiss, E. Tóth-Kádár, A. Dinia*, V. Pierron-Bohnes*, I. Bakonyi: Giant magnetoresistance and magnetic properties of electrodeposited $Ni_{81}Cu_{19}$/Cu multilayers. *J. Magn. Magn. Mater.*, accepted for publication (see also D.15.)

I.12. A. Vértes*, K. Süvegh*, M. Bokor, A. Domján*, T. Marek, M. Klapper*, C.U. Chisholm*, M. El-Sharif*, K. Tompa, Zs. Nemes-Vetéssy*, K. Burger*: Frontiers of positron and positronium chemistry in condensed media. *J. Radioanal. Nucl. Chem. Articles*, accepted for publication

Conference proceedings:

I.13. M. Bokor, T. Marek, K. Tompa, A. Vértes*: Anion dynamics in tetrafluoroborate salts of Zn^{II}- and Fe^{II}-propyltetrazole complexes. In: *Proc. Joint 29th AMPERE — 13th ISMAR Int. Conference (Berlin, 1998).* D. Ziessow, W. Lubitz and F. Lendzian (eds.), Vol. I., pp. 617-618.

I.14. Á. Cziráki*, I. Bakonyi: Common features of the microstructure in the multilayers. In: *Proc. 14th Int. Congress on Electron Microscopy (Cancun, Mexico, 1998).* Eds. H.A. Calderón Benavides and M. José Yacamán (Institute of Physics Publishing, Bristol and Philadelphia, 1998), Vol. II, pp. 317-318.

I.15. A. Lovas, J. Garaguly: The role of hydrogen-energetics in the future of transportation industry. In: *Gépészet '98, Proc. of 1st Conf. on Mechanical Engineering (Budapest, 1998).* Eds. K. Molnár, Gy. Ziaja and G. Vörös (Springer Hungarica Kiadó, Budapest, 1998), pp. 692-696. (see also J.19.)

I.16. T. Marek, M. Bokor, K. Tompa, A. Vértes*: Solid-state ^{1}H and ^{19}F NMR spectroscopic study of iron(II) alkyltetrazole spin-crossover compounds. In: *Proc. Joint 29th AMPERE — 13th ISMAR Int. Conference (Berlin, 1998).* D. Ziessow, W. Lubitz and F. Lendzian (eds.), Vol. II., pp. 683-684.

I.17. L. Pogány, I. Varga, C. Hargitai, Z. Fülöp*, I. Bakonyi: Simulation of the deflection of electron trajectories due to domain magnetization. In: *Proc. 14th Int. Congress on Electron Microscopy (Cancun, Mexico, 1998).* Eds. H.A. Calderón Benavides and M. José Yacamán (Institute of Physics Publishing, Bristol and Philadelphia, 1998), Vol. I, pp. 1677-168. (see also J.20.)

I.18. K. Tompa, P. Bánki, J. Garaguly, G. Lasanda, L. Vasáros*: Partition of hydrogen in Ni-Zr-H alloys. In: *Proc. Joint 29th AMPERE — 13th ISMAR Int. Conference (Berlin, 1998).* D. Ziessow, W. Lubitz and F. Lendzian (eds.), Vol. I., pp. 172-173.

I.19. I. Varga, L. Pogány, C. Hargitai, I. Bakonyi: Domain wall movement on $Fe_{85}B_{15}$ investigated by stroboscopic SEM. In: *Proc. 14th Int. Congress on Electron Microscopy (Cancun, Mexico, 1998).* Eds. H.A. Calderón Benavides and M. José Yacamán (Institute of Physics Publishing, Bristol and Philadelphia, 1998), Vol. II, pp. 557-558. (see also J.22.)

Book chapter:

I.20. K. Tompa: Nuclear magnetic resonance in geosciences. In: *Nuclear Methods in Mineralogy and Geology. Techniques and Applications*. Eds. A. Vértes, S. Nagy and K. Süvegh (Plenum Press, New York, 1998), pp. 251-284

Others:

I.21. P. Rácz*, P. Bánki, C. Hargitai, G. Lasanda, K. Tompa: Proton spin-spin relaxáció emberi normál és öregkori szürke hályogos, tiszta hal és madár szemlencséken (Proton spin-spin relaxation in normal and cataractous human, normal fish and bird eye lenses, in Hungarian). *Szemészet (Budapest)* **134**, 25-29 (1997)

I.22. M. Bokor, K. Süvegh*, K. Tompa, A. Vértes*: Hidrogéntároló Pd-Ag ötvözet vizsgálata pozitronannihilációs spektroszkópiával (Study of hydrogen-storing Pd-Ag alloy by positron annihilation spectroscopy, in Hungarian) (abstract). In: *Programme Booklet of the Conference " Radiochemistry Autumn Days '98" (Õszi Radiokémiai Napok '98, 1998, Paks, Hungary)*

I.23. P. Rácz*, B. Alföldy, P. Bánki, C. Hargitai, K. Tompa: ^{1}H NMR spin-spin relaxation in normal and cataractous human, normal fish and bird lenses (abstract). In: *Proc. XIIIth International Conference on Eye Research (Paris, 1998)*

J. METALLURGY AND MAGNETISM

L.K. Varga, A. Kákay[+], P. Kamasa, G. Konczos, A. Lovas[++], J. Pádár, L. Pogány, F.I. Tóth, B. Varga[+++], I. Varga[++++]

Soft magnetic nanocrystalline alloys. — We have continued the systematic study of both Finemet ($Fe_{73.5-x}Cr_xSi_{13.5}B_9Nb_yCu_1$, with x = 0, 6, 8, 10, 12 and y = 1, 3, 5) and Nanoperm ($Fe_{92-x}Zr_{7-y}B_xNb_yCu_1$, with x = 2,4,6,8,10,12 and y=0, 3.5) type soft magnetic nanocrystalline alloys. By comparative initial permeability (μ_i) and low field dc magnetization (M_s) measurements, it is demonstrated that the two-phase system (bcc nanograins and residual amorphous phase) shows a sequence of magnetic phase transformations as a function of temperature. Below the Curie point of the initial amorphous state, a rounded Hopkinson peak is observed in the initial permeability versus temperature curve. Below this Hopkinson peak, the bcc nanograins are pertfectly coupled through the ferromagnetic amorphous matrix. Above it, however, the bcc nanograins are gradually decoupled as the increasing temperature gradually surpasses the Curie temperatures of all the coupling amorphous spacers with slightly differring chemical compositions. The weakened coupling results in an increase of the effective crystalline anisotropy which affects all the magnetic characteristics: the material becomes gradually hardened, i.e,. the coercive field starts increasing and the initial permeability decreasing; the domain structure changes from wide domains to a pattern of small irregular domains. Above the Curie point of the amorphous matrix, the coupling between the nanograins is not completely interrupted but still persists to the next temperature interval characterized by a "superferromagnetic" state. In this state, a residual coupling exists which can be either exchange or dipolar or both and it depends sensitively on the annealing conditions, i.e., on the crystalline fraction. At a given fraction, i.e., at a given distance between the grains, the strength of the interaction decreases with increasing temperature due to the simultaneous decrease of magnetization in the bcc nanograins until thermal energy dominates and the magnetization behaviour becomes superparamagnetic. At this transition (T_{sf}), the system is again magnetically soft and a second peak in the initial permeability thermogram can be observed. The magnetization versus temperature curve, however, shows no specific feature at T_{sf}, and disappears at a higher temperature called superparamagnetic-paramagnetic transition (T_{sp}) which is dependent on the applied d.c. field. This T_{sp} transition temperature will coincide with the Curie temperature of nanograins at very large measuring field only. Tailoring of new two-phase (or even better, monophase, if possible) nanocrystalline soft magnetic materials is necessary to increase the T_c of the matrix responsible for the ferromagnetic coupling between the bcc nanoparticles and to prepare in this way new materials applicable at high temperatures as well. The applicability of Cr-doped Finemet alloys for magnetocaloric effect is under investigation.

Metal-hydrogen systems. — A feasibility study of the reversible storage of hydrogen in intermetallic alloys has been prepared for the Hungarian Branch of LINDE Company (Répcelak). It is concluded that for reversible storage in small sparklet for fuel cell applications, an AB_5 type alloy in nanocrystalline state is an appropriate

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choice. An equipment was proposed based on mass flowmeter and constant pressure regulator in order to perform absorption and desorption kinetic tests under isothermal and isobaric conditions.

Scanning electron microscopy (SEM) studies. — The most significant result was the development of a new attachement for the investigation of domain movement in soft magnetic materials. This new attachment is able to show the domain movement on metallic ribbons and on the same sample material, we can measure in-situ the histeresys loop and permeability of the sample. An ananlysis of ion distribution in arbuscular micorrhysas was made on dry fungi samples but for more realistic results, there is a need for developing a new technique for sectioning. Morover, the real ion distribution can change during the sectioning process and, therefore, the samples should be frozen and kept cooled during sectioning by thinning. The sample thinning will be performed by a newly purchased ion milling gun which is now being installed in the laboratory. This ion milling equipment will also be used for preparing TEM cross-sectional samples of magnetic multilayers. Significant development has been achieved recently in the laboratory hardware and software used for the evaluation of SEM experimental results (qualitative and quantitative evaluation of electron microsonde spectra for the chemical analysis of thin layers and evaluation and archiving of the electron microscopic pictures).

Development of a digital phase-sensitive detector. — Based on the digital signal processing (DSP) technique, a digital phase sensitive detector (DPSD) has been developed and built. This type of instruments is widely used in research by applying continuous-wave modulation where a major requirement is to detect small-amplitude modulated signals immersed in noise.The new instrument has already found an application in Auger Electron Spectroscopy and has been installed at the Research Institute for Technical Physics and Materials Science of the HAS. The high performance of the DPSD was verified in several other measurements including: thermomagnetic measurements, nuclear and electron magnetic resonance spectroscopy, spectrophotometry and nondestructive testing.

Development of magnetoresistance measuring equipment. — Since the discovery of the so-called "giant" magnetoresistance, there has been a large interest, both from practical and fundamental point of view, in developimg a general-purpose technique for the measurement of magnetoresistance of magnetic/nonmagnetic metallic multilayers. The magnetoresistance is mostly measured by applying four point contacts to the sample. However, with this technique the measurement often suffers from the shunting effect of the metallic seed and/or cover layers, unless the multilayer can be removed from the substrate which cannot be performed for very thin multilayers. In order to circumvent these problems, we have designed and constructed an equipment for the contactless electronic measurement of resistance for routine testing which can provide considerable advantages over the standard technique. By placing the sample into the coil of a marginal oscillator which is operated at the resonant condition, changes in the impedance of the sample can be measured, similarly to a conventional AC impedance measurement, as a function of the magnetic field.

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Grants

OTKA T020891 Study of intracellular element distribution in soil microorganisms (L. Pogány, 1996-1999)
GE-TUNGSRAM: Contract for materials research by SEM (L. Pogány, 1998)
AGMI (Material Testing and Quality Control Co.): Contract for design and construction of eddy-current probe for non-destructive testing of high-pressure chemical reactor walls at Tisza Chemical Works (TVK) (P. Kamasa, 1998)
Linde Gas Hungary Co.: Hydrogen storage in metal hydrides (state-of-the-art study) (L.K. Varga, 1998)

Publications

Articles

J.1. Á. Böhönyey*, G. Huhn*, L.F. Kiss, A. Lovas, I. Gerõcs*: Effect of metalloid substitution on the reversible structural relaxation of Fe-Ni-B(-P,Si) metallic glasses. *J. Non-Cryst. Sol.* **232-234,** 490-496 (1998) (see also D.7)

J.2. I. Jacyna-Onyszkiewicz*, P. Kamasa: Magnetic domain behaviour of Cu-ferrite doped with small quantities of Cd or Be ions. *J. Phys. IV (France)* **8**, Pr2/315-318 (1998)

J.3. T. Kemény, L.K. Varga, L.F. Kiss, J. Balogh, T. Pusztai, L. Tóth*, I. Vincze: Magnetic properties and local structure of Fe-Zr-B-Cu nanocrystalline alloys. *Mater. Sci. Forum* **269-272**, 419-424 (1998) (see also D.2.)

J.4. A. Lovas, L.F. Kiss, B. Varga, P. Kamasa, I. Balogh, I. Bakonyi: Survey of magnetic properties during and after amorphous-nanocrystalline transformation. *J. Phys. IV (France)* **8**, Pr2/291-298 (1998) (see also D.8 and I.4)

J.5. L. Pogány, D.T. Son*, I. Varga, Z. Fülöp*, C. Hargitai, I. Bakonyi: Measurement of internal magnetic domain structures by using backscattered electrons in a SEM. *J. Phys. IV (France)* **8**, Pr2/697-700 (1998) (see also I.5.)

J.6. F. Sommer*, T. Tarnóczi, K. Russew*, Á. Cziráki*, L.F. Kiss, L.K. Varga, I. Bakonyi: Preparation, structure and physical properties of Fe-, Co- and Ni-rich melt-quenched ribbons containing Zr or Hf. Part IV: Thermal stability: DSC, TEM and thermomagnetic studies. *Z. Metallkde.* **89**, 256-266 (1998) (see also D.9 and I.6.)

J.7. B. Varga, J. Takács*, A. Lovas, P. Kamasa, F. Zhou*, J. Vandlik*: Comparison of the thermomagnetic and thermal effects during nanocrystallization of $Fe_{76.5-x}Cu_1Nb_xSi_{13.5}B_9$ glassy precursors. *J. Mater. Sci. Technol.* **14**, 323-326 (1998)

J.8. L.K. Varga: Thermal behaviour of the initial permeability in soft magnetic nanocrystalline alloys. *J. Phys. IV (France)* **8**, Pr2/55-58 (1998)

J.9. L.K. Varga D. Kaptás, T. Kemény: Soft magnetic nanocrystalline powders obtained by mechanical grinding. *Mater. Sci Forum* **269-272**, 731-736 (1998) (see also D.3.)

J.10. R. Varga*, P. Vojtanik*, A. Lovas: Time and thermal stability of magnetic properties of amorphous $Fe_{80}TM_3B_{17}$ alloys *J. Phys. IV (France)* **8**, Pr2/63-66 (1998)

J.11. J. Zbroszczyk*, L.K. Varga, J. Olszewski*, H. Ciurzynska*: Magnetic properties and Mössbauer studies of $Fe_{86}Zr_7B_6Cu_1$ alloy. *J. Phys. IV (France)* **8**, Pr2/203-206 (1998)

J.12. I. Bakonyi, E. Tóth-Kádár, J. Tóth, L. Pogány, T. Tarnóczi, P. Kamasa: Magnetic and electrical transport properties of electrodeposited Ni-Cu alloys and $Ni_{81}Cu_{19}$/Cu multilayers. submitted to *J. Phys. Cond. Matter* (accepted for publication) (see also I.8.)

J.13. D. Garcia*, G.V. Kurlyandskaya*, M. Vázquez*, F.I. Tóth, L.K. Varga: Influence of field annealing on the hysteretic behaviour of the giant magneto-impedance effect of Cu wires covered with $Ni_{80}Fe_{20}$ outer shells. *J. Magn. Magn. Mater.* (accepted for publication)

J.14. P. Kamasa, P. Myśliński*, B. Varga, Z. Jurasz*: Investigation of the oxidation process in rod and foil samples of iron samples by thermomagnetic measurements. *acta phys. slovaca* (accepted for publication)

J.15. V.T. Lebedev*, G.P. Gordeev*, A.I. Sibilev*, V.V. Klyubin*, Gy. Torok, L. Cser, Gy. Kali, L.K. Varga, A. Brulet*: Neutron spin echo study of low-T_c ferrofluid. *J. Magn. Magn. Mater.* (accepted for publication) (see also K.21.)

J.16. A. Sólyom*, P. Marko*, P. Petrovic*, D. Matisová*, G. Konczos: Rapidly quenched microcrystalline FeSiCo alloys.. *acta phys. slovaca* (accepted for publication)

J.17. R. Varga*, P. Vojtaník*, J. Kovác*, P. Agudo*, M. Vazquez*, A. Lovas: Influence of Cr on magnetic and structural properties of amorphous $Fe_{80-x}Cr_xSi_6B_{14}$ (x=0-14) alloys. *acta phys. slovaca* (accepted for publication)

Conference proceedings

J.18. P. Kamasa, J. Duchiewicz*: Digital phase-sensitive detector using Gabor transform. In: *Proc. XXXth Polish Seminar on NMR* (Cracow, 1997). Institute of Nuclear Physics (Cracow, 1998), pp. 201-204

J.19. A. Lovas, J. Garaguly: The role of hydrogen-energetics in the future of transportation industry. In: *Gépészet '98, Proc. of 1st Conf. on Mechanical Engineering (Budapest, 1998).* Eds. K. Molnár, Gy. Ziaja and G. Vörös (Springer Hungarica Kiadó, Budapest, 1998), pp. 692-696. (see also I.15.)

J.20. L. Pogány, I. Varga, C. Hargitai, Z. Fülöp*, I. Bakonyi: Simulation of the deflection of electron trajectories due to domain magnetization. In: *Proc. 14th Int. Congress on Electron Microscopy (Cancun, Mexico, 1998).* Eds. H.A. Calderón Benavides and M. José Yacamán (Institute of Physics Publishing, Bristol and Philadelphia, 1998), Vol. I, pp. 1677-168. (see also I.17.)

J.21. A. Sólyom*, P. Marko*, A. Lovas: Microcrystalline Fe-Si-Co ribbons prepared by rapid solidification. In: *Proc. 10th Int. Symp. on Metallography (Tatranska Lomnica, Slovakia, 1998).* pp. 512-513

J.22. I. Varga, L. Pogány, C. Hargitai, I. Bakonyi: Domain wall movement on $Fe_{85}B_{15}$ investigated by stroboscopic SEM. In: *Proc. 14th Int. Congress on Electron Microscopy (Cancun, Mexico, 1998).* Eds. H.A. Calderón Benavides and M. José Yacamán (Institute of Physics Publishing, Bristol and Philadelphia, 1998), Vol. II, pp. 557-558. (see also I.19.)

K. NEUTRON SCATTERING IN CONDENSED MATTER

L. Rosta, L. Almásy, S. Borbély, L. Cser, T. Grósz, P. Jóvári, L. Kõszegi, E. Rétfalvi, L. Riecsánszky, Gy. Török

The Budapest Research Reactor. — Our Institute is one of the three associates of the Budapest Neutron Centre operating and using the 10 MW *Budapest Research Reactor (BRR)* on the KFKI site. This modern neutron source - with its unique possibilities in Central Europe - is open for the international user community and serves various tasks, such as basic and applied research in physics, chemistry, biology, materials science, as well as commercial utilisation and education. For neutron beam measurements different types of horizontal channels are available: seven thermal and two fast neutron channels; a tangential beam tube serves for the neutron guide system. The Neutron Physics Department on one hand operates several experimental stations located on the above beam-lines, on the other hand provides services for external users to perform experiments and exploit the obtained results. In 1998 nearly 40 experiments were completed by the local staff and in collaboration with national or foreign users coming from university, industrial or other research laboratories.

We operate at BRR a pine-hole collimation type *small angle neutron scattering* (SANS) instrument and a *triple axis spectrometer* (TAS) both installed on neutron guides. A new reflectometer is in use since the beginning of 1998. The installation of another TAS instrument and a *4-circle materials test diffractometer* has been started on thermal neutron beams. Our activity related to neutron scattering is based essentially on experiments performed on the above spectrometers, some special studies, however, were performed at other neutron source facilities e.g. at Saclay (France) where we shared the construction of the Spin-Echo spectrometer (or at HMI Berlin, FLNP Dubna, IRI Delft).

Our team is mainly interested in condensed matter research: the investigation of structure and dynamics of *liquids* (e.g. various solutions and anisotropic fluids) and *soft materials*, as well as material properties of *solids* (like metals, alloys, composites etc). In the followings a few examples of this activity will be shortly described.

Liquids. — The small angle scattering investigation of *polymer solutions* has substantial impact on chemical, pharmaceutical industry. We have studied a particular system, the interaction between EO-PO-EO type triblock copolymer Pluronic F68 and perdeuterated o-xylene in aqueous solutions. The o-xylene is a selective solvent for the poly(propylene oxide) middle block. The measurements revealed that the interaction between the polymer and the additive promote the temperature induced aggregation of polymer molecules. The effect depends on the polymer concentration, temperature and on the additive-to-polymer molar ratio, and shows a saturation behaviour with increasing amount of o-xylene.

Results of neutron diffraction experiments have been modelled by the reverse Monte Carlo (RMC) method applied to microscopic investigations on the structure of *simple molecular liquids* (CS_2, Cse_2). This work has revealed that orientational correlation vanishes if the distance of molecules is greater than 6Å, that is angular correlation exists only between nearest neighbours. CS_2-Tetramethylurea *(TMU) mixtures* have also been studied by neutron diffraction. According to the model structures obtained

by RMC the formation of contact TMU pairs is significant in the solutions investigated.

Structural transitions were studied in *frozen ferrous perchlorate solution*. Quenching a liquid solution typically gives rise to metastable solid phases, which can transfer to more stable states via ageing, heating or other procedures. In a previous work quenched ferrous perchlorate was investigated using Mössbauer-effect. A phase transition was found, where the frozen amorphous sample before the crystallisation passes through a viscous-like state. By small-angle neutron and X-ray scattering, and neutron diffraction the different structures were studied, the existence of an amorphous (viscous) re-entrant phase was clearly demonstrated and a model of the process is constructed, which allows to explain the experimental results.

The dynamical behaviour *of various ferrofluids* were investigated by the use of neutron spin-echo technique. The interference between the nuclear and magnetic scattering allowed to separate the molecular diffusion and the spin dynamics. It was found a strong density fluctuation near $T_c \approx 20°C$ and H=0, induced by critical spin diffusion. The temperature variation of the self correlation function $G_s(T,q,t) = \exp[-q^2D\cdot(t/\tau)^{\beta(T)}]$ at momentum transfer $q = 0.07Å^{-1}$ in the time interval t = 0.5 - 40ns reveals strong influence of magnetic fluctuations on the mobility of the system. Using isotopic labelling strong influence of dipole forces on the motion of a particle was observed. It resembles the segmental relaxation in a polymer chain. On the other hand, the pair correlation reveals oscillation character.

Soft materials. — Magnetic phase ordering in *ferrogels* under applied field was also studied. A new cross linked polymer compound (hydrogel) containing fine Fe_3O_4-grains has been investigated by neutron scattering. We have studied the nanoscale structures of these ferrogels synthesised in a magnetic field and without a magnetic field. By means of polarised neutron scattering we studied the self-assembly of the particles under the influence of the magnetic field. Even in a weak field (H~65Oe) the ferrogel showed strong spatial correlation of the particles; a strong field (H~4kOe) induced slow growth of the interference effect.

The influence of cyclic thermal treatment near the first order phase transition on the *supramolecular structure of* C_{60} was studied by neutron diffraction and small angle scattering. The fragmentation of surface structures at the scale of ~10nm was observed. From the small-angle neutron scattering data the corresponding fractal dimension was determined. The fractal dimension value depends on the stage of the thermal treatment.

Interpenetrating network based *polymer membranes* have great interest in the food and pharmaceutical industry. Neutron scattering study on such materials was carried out by using the small-angle scattering technique. The obtained results confirm the high thermal stability of membranes. Two characteristic scales of pores in membranes were found (~30 nm and ~2 nm size) being responsible for high filtering properties of this molecular sieve.

Solids. — The results of systematic measurements using anisotropic SANS method on a series of doped *tungsten* rods and wires revealed quantitative information on average deformation of potassium bubbles during the thermomechanical treatment procedure, namely the proper ratio of numbers of elongated ellipsoids and spheres can be assigned to the given steps of the treatment.

The apparent grain size of milled *nanocrystalline tungsten-carbide powder* samples determined by SANS is significantly greater, compared to results of measurements by

other methods, because the SANS method also reveals the surface of agglomerates of closely packed grains. The rate of decrease of internal surface during sintering was investigated on WC-Co hard metal samples. It is worthy to note that, similarly to findings by others, no drastic internal surface decrease was observed at 1330 °C temperature, the bulk melting point of Co based binding phase indicating that in nanostructure the melting of binding phase begins at a lower temperature.

Internal stress measurements were performed in Saclay. The main programme in this field is the stress investigations on the grain boundaries. In the last period we extended our investigations to non-ambient temperatures. As a first step the measurements were started at above room temperature. The main task was to determine how the temperature variation influences stresses on the grain boundary.

Surface and layer structure studies were primarily related to the start-up operation of a preliminary reflectometer assembly installed on a neutron guide. Valuable results were obtained in porous silicon samples, a surface layer of about 30 nm was found. The layer thickness seems to coincide with the diameter range of the tubular pores of the sample and thus the surface layer may be attributed to the roughness caused by the craters of the tubular pores. Another study revealed structural changes in C_{60} fulleren deposited layers. The samples were annealed and the comparison of the reflectogrammes before and after annealing shows that the annealed layers are much smoother, their thickness appears to be more homogeneous.

Instrumentation development. — In order to maintain a high level experimental research capacity at modest financial frames, we devote special efforts to enhance neutron beam intensity and develop various neutron scattering instrument components. The major current development at BRR is the installation of a cold moderator for expanding our condensed matter research possibilities for the highly demanded *cold neutron* region. The main component of the liquid hydrogen Cold Neutron Source have been manufactured and purchased. We are ready to assemble the CNS system at the beginning of next year. For the improved transportation of the neutron beams multilayer neutron optical elements (e.g. supermirrors) are developed in collaboration with a small business company equipped with a large magnetron sputtering station.

On the spectrometer development side the following examples are worth mentioning. To provide monochromatic beams in the long wavelength range we have developed and patented a multidisc type *velocity selector*. The upgrading of its construction is in progress now. On the detection side we have launched a program for equipping our instruments with multiwire gas chamber *area detectors* with the proper electronic and data acquisition system.

Meetings. **—** Since 1993 the Neutron Physics Department organises regularly an international autumn meeting either with workshop character (to initiate, for instance, a topical project or instrument construction) or for training purposes. This year the title was *„International School and Symposium on Small-angle Scattering"* and the meeting was held from 8^{th} to 11^{th} October in the resthouse of the Hungarian Academy of Sciences at Mátraháza. More than 50 participants, nearly the half from Hungary and the rest from abroad (16 countries), attended the Meeting. Seven invited lectures was delivered by internationally reknown experts of small-angle scattering tecnique. These lectures covered the basic ideas of the method and its applications in different fields of sciences. Moreover, short lectures were held by the participants presenting their own results. One should note that the major part of the attendies was young scientists, graduate and Ph.D. students, mainly from Hungary.

The annual meeting of the *International Scientific Advisory Council* of the Budapest Neutron Centre took place on the 10th of October. It was started with an open session by a scientific lecture on the use of neutron scattering in biology given by P. Timmins (ILL Grenoble). The Council - among others - endorsed with satisfaction the succesful multidisciplinary use of our SANS machine and stressed on the importance of the upgrade of the neutron guide system in conjunction with the cold source installation.

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Grants

AKP 96/2-406 2,2	Investigation of phase transitions in metastable systems (L. Cser, 1996-98)
EU CIPA CT92-4011	Neutron scattering in molecular systems (L. Rosta, 1993-98)
EU ERB-CT96-0057	Perfect crystal neutron optics (L. Rosta, 1997-2000)
EU ERB-CT98-0098	Cold neutron optimisation (L. Rosta, 1998-2001)
EU ERB PL96-9007	Neutron Round Table (L. Rosta, 1998-2001)
IAEA 75214/HUN	Condensed matter research (L.Cser, 1996-1998)
OMFB 0478/97	High speed velocity selector development (L. Rosta, 1997-1999)
OMFB EO 097/97	Perfect crystal neutron optics (L. Rosta, 1997-2000)
OMFB EU-97-B4-98	Cold neutron optimisation (L. Rosta, 1998-2001)
OMFB EI-65/98	Neutron beam sources (L. Rosta, 1998-2000)
OTKA T 025747	Structure of polymer solution by small angle neutron scattering (S. Borbély, 1998-2001)
OTKA T 17016	Ordering phenomena in interface and surface thin layers (L. Cser, 1995-98)
OTKA T 22486	Investigation of sintering processes using neutron scattering methods (T.Grósz, 1997-2000)
OTKA T 16943	Decomposition of liquid crystal based binary systems (L. Rosta, 1995-98)

Publications

Articles

K.1. L. Almásy, A. Jákli, L. Rosta, G. Pépy*: Structural Memory Effect in Liquid Crystal Phases Stabilised by Silica Particle Aggregates. *Physica* **B 241-243**, 996-998 (1998) (see also G.1.)

K.2. L. Kõszegi: Internal stresses on precipitated Cu-grains in the Fe-Cu alloy. *Physica* **B 241-243**, 1258-1260 (1998)

K.3. A.V. Belushkin*, M. Bull*, C. Carlile*, S.G. Lushnikov*, L. Rosta, L.A. Shuvalov*, Gy. Török, B.T.M. Willis*: Inelastic neutron scattering in a $Cs_5D_3(SO_4)_4$ crystal. *Physica* **B 241-243**, 484-486 (1998)

K.4. Gy. Mészáros, L. Almásy, E. Sváb, L. Cser, I. Dézsi*: Neutron diffraction study of frozen $Fe(ClO_4)_2$ solutions. *Materials Science Forum* **278-281**, 732-737 (1998) (see also D.10.)

K.5. S. Borbély: Small-angle neutron scattering study of Pluronic F68 tri-block copolymer solutions. *Physica* **B 241-243**, 1016-1018 (1998)

K.6. T.Grósz, L.Bartha*, S.Borbély, P. Harmath*, L.Rosta: SANS investigation of sintering process based on nano-crystalline powder. *Physica* **B 241-243**, 350-351 (1998)

K.7. L.Cser, G.Jancsó*, P.Jóvári, Gy.Káli: Temperature dependence of small angle neutron scattering of tetramethylurea in carbon disulfide solution. *J.Phys.Chem.***B 102**, 2313-2316 (1998)

K.8. V.T. Lebedev,* G.A. Evmenenko*, V.L. Alekseev*, D.M. Orlova*, Gy. Török, L. Cser, V.N. Zgonnik*, V.P. Budtov*, A.A. Polyakov*, V.V. Klyubin*, A.I. Sibilev*, M.A. Sibileva*: Associations of fullerene-containing PVP in water solutions (in Russian). *Zhurnal Vysokomolekularnyh Soedinenij*, accepted for publication

K.9. V.T. Lebedev*, G.A. Evmenenko*, V.L. Alexeev*, D.M. Orlova*, Gy. Török, L. Cser, V.V. Klyubin*, A.A. Polyakov*, V.P. Budtov*, P.N. Moskalev*, A.I. Sibilev*, M.A. Sibileva*: Structure of complexes of poly-N-vynilpyrrolidone with diphtalocyanides of rare earth elements in D2O solutions (in Russian). *Zhurnal Vysokomolekularnyh Soedinenij*, accepted for publication

K.10. V.T. Lebedev*, Gy. Török, L. Cser, A.L. Buyanov*, L.G. Revelskaya*, A.I. Sibilev*, D.N. Orlova*: Polarized neutron study of magnetic ordering in ferrogels (in Russian). *Kolloidnyj Zhurnal*, accepted for publication

K.11. P. Jóvári: On the separation of inter and intramolecular elastic neutron scattering intensities: the case of liquid CS_2. *Mat. Sci. Forum*, accepted for publication.

K.12. V.T. Lebedev*, Gy.Török, G.A.Evmenenko*, I.V. Golosovsky*, Gy. Káli, L. Cser, A. Brulet*, D.N. Orlova*, A.I. Sibilev*, V.P. Budtov*: Influence of cyclic

thermal treatment near the first order phase transition on the supramolecular structure of C_{60}. *Mat. Sci. Forum*, accepted for publication.

K.13. Gy. Török, V.T. Lebedev*, L. Cser, A.L. Buyanov*, L.G. Revelskaya*: Neutron scattering study of polymer membranes based on interpenetrating network. *Mat. Sci. Forum*, accepted for publication

K.14. V.T. Lebedev*, G.A. Evmenenko*, V.L. Akexeev*, D.N. Orlova*, Gy.Török, L. Cser, V.N. Zgonnik*, L.A. Vinogradova*, E.N. Melelevskaya*, E.E. Kever*, V.P. Budtov*, A.A. Polyakov* ,V.V .Klyubin*, A.I. Sibilev*, M.A. Sibileva*: Study of polivinilpyrrolidone-C_{60} complex in water solution by neutron and light scattering and viscosimetry. *Mat. Sci. Forum*, accepted for publication

K.15. V.T. Lebedev*, Gy. Török, L. Cser, A.L. Buyanov, L.G. Revelskaya, D.N. Orlova, A.I. Sibilev**:** Magnetic Particle Structure Ordering in Ferrogel Under Applied Magnetic Field. *Mat. Sci. Forum*, accepted for publication

K.16. V.T. Lebedev*, Gy. Török, L. Cser, A.L. Buyanov*, L.G. Revelskaya*, D.N. Orlova*, A.I. Sibilev*: Magnetic phase ordering in ferrogels under applied magnetic field. *Journal of Magnetism and Magnetic Materials*, accepted for publication

K.17. V.T. Lebedev*, Gy. Török, Gy. Káli, L. Cser, A. Brulet*, D.N. Orlova*, A.I. Sibilev*: Dynamics of concentrated ferrofluids with labelled particles: *Journal of Magnetism and Magnetic Materials*, accepted for publication.

K.18. Gy. Kádár*, É. Vázsonyi*, S. Borbély, Gy. Káli: Small-angle neutron scattering in P+ doped porous silicon. *J.Porous Mat.*, accepted for publication.

K.19. S. Gierlotka*, B. Palosz*, R. Pielaszek*, S. Stel'makh*, S. Borbély, D.G. Keil*: Neutron and X-ray investigations of crystallite and particle size distribution in nanometric silicon carbide. *Mat. Sci. Forum*, accepted for publication.

K.20. A.M. Kiselev*, M.A. Kiselev*, S. Borbély, P. Lesieur*: Influence of ethanol on the membrane structure: SANS study. *Mat. Sci. Forum*, accepted for publication.

K.21. V.T. Lebedev*, G.P. Gordeev*, A.I. Sibilev*, V.V. Klyubin*, Gy. Török, L. Cser, Gy. Káli, L.K. Varga: Neutron spin echo study of low-Tc ferrofluid. *Journal of Magnetism and Magnetic Materials*, accepted for publication (see also J.15.)

Conference proceedings

K.22. L. Rosta: The Budapest Experience for Installation of Liquid Hydrogen Moderator and Guide Equipment for Neutron Scattering Research. In: *Proc. Int. Workshop on Cold Neutron Utilisation*, Taejon, Korea; KAERI/GP-119/98, 63 (1998)

K.23. L. Bartha*, P. Harmat*, O. Horacsek*, T. Grósz, L. Rosta: Neutron scattering method for analysis of nanosized inclusions in tungsten. In: *Proc. Int. Regional*

Workshop, Science, Technology, Development, Uzhgorod, May 29-30, 1998, pp. 13-22.

K.24. L. Cser, L. Rosta, Gy. Kaszás*, Th Krist*, F. Mezei: Investigation of Neutron Optical Multilayer Systems. In: *Proc. Conf. on Materials Research Using Cold Neutrons at Pulsed Neutron Sources,* Argonne, 1997, accepted for publication

K 25. T. Grósz, P. Harmat*, O. Horacsek*, L. Rosta: Small Angle Neutron Scattering Study of Oriented Dispersoids in Tungsten Wire. In: *Proc. Conf. on Materials Research Using Cold Neutrons at Pulsed Neutron Sources,* Argonne, 1997, accepted for publication

K.26. L. Rosta: Cold Neutron Source Development and Industrial Oriented Research at the Budapest Neutron Centre. In: *Proc. Conf. on Materials Research Using Cold Neutrons at Pulsed Neutron Sources,* Argonne, 1997, accepted for publication

K.27. L. Bartha*, P. Harmat*, O. Horacsek*, T. Grósz, L. Rosta: Characterisation of second phase dispersoids of doped tungsten wire by means of small angle neutron scattering. In: *Proc. Int. Conf. on Tungsten, Refractory Metals and Alloys*: *Processing, Properties and Applications* Nov.16-19, 1997, Orlando, Florida, USA, accepted for publication

K.28. M.A. Kiselev*, L.I. Barsukov*, S. Borbély, A.M. Kiselev*, S.A. Kutuzov*: Investigation of the Temperature Induced Micelle to Lamellar Transition via Small Angle Neutron Scattering. In: *Proc. of XV Int. Workshop on the Applications of Neutron Scattering to Solid State Physics*, March 17-23, 1998, Zarechny, Russia, accepted for publication

K.29. L. Cser: Organical compounds for cold moderators. In: *Proc. Int.* W*orkshop on cold moderators for pulsed neutron sources*, 28 Sept.-02 October,1997. Argonne National Laboratory, USA, accepted for publication

K.30. A.M. Kiselev*, M.A. Kiselev*, S. Borbély, L.I. Barsukov*, M. Ollivon*, P. Lesieur*: Temperature Induced Micelle to Vesicle Transition as Studied by Neutron and X-ray Small Angle Scattering. In: *Proc. of NATO ASI Workshop on Dynamical properties of unconventional magnetic systems,* April 2-12, 1998, Gielo, Norway. IFE/KR/E-97/005, Institute for Energy Technology, accepted for publication

K.31. M.A. Kiselev*, A.M. Kiselev*, S. Borbély, P. Lesieur*: Influence of Ethanol on the Membrane Structure: SANS study. In: *Proceedings of International Workshop on Deuteration of Biological Molecules for Structural and Dynamical Studies. Applications to Neutron Scattering and NMR*. May 19-25, 1998, Dubna, Russia. (accepted for publication)

K.32. L. Rosta: Progress and Experience on Neutron Research Development in Hungary after the Restart of the Upgraded Budapest Research Reactor. In: *Proc. of the "Workshop on Instrumentation for the AUSTRON project"* Vienna, June30-July1, 1998, accepted for publication

K.33. S. Borbély: SANS from Brij35-SDS mixed solutions. In: *Proc. Int. School and Symposium on Small-Angle-Scattering*, October 8-11, 1998, Mátraháza, Hungary, accepted for publication

K.34. L. Cser: Small Angle Neutron Scattering Instrumentation. In: *Proc. Int. School and Symposium on Small-Angle-Scattering*, October 8-11, 1998, Mátraháza, Hungary, accepted for publication

K.35. P. Harmat*, O. Horacsek*, T. Grósz, L. Rosta: SANS investigation of sintered material: doped, sintered, deformed tungsten containing K bubbles. In: *Proc. Int. School and Symposium on Small-Angle-Scattering*, October 8-11, 1998, Mátraháza, Hungary, accepted for publication

K.36. P. Harmat*, L. Bartha*, T. Grósz, L. Rosta: Investigation of Internal Surfaces of WC-Co Composites using Small Angle Neutron Scattering. In: *Proc. Powder Metallurgy'*98 *Special Interest Seminar on Hard Materials*, 16-20 October 1998, Granada, Spain, accepted for publication

K.37. L. Cser: PC-based data acquisition in solid state research using neutrons at the Budapest Neutron Centre. In: *Proc. IAEA technical committee meeting on improvement of the data acquisition for research reactors and experiments*. 19-21 October, 1998, Pitesti, Romania, accepted for publication

Others

K.38. V.T. Lebedev*, G.A .Evmenenko*, V.L. Alekseev*, D.M. Orlova*, Gy. Török, L. Cser, V.N. Zgonnik*, V.P. Budtov*, A.A. Polyakov*, V.V. Klyubin*, A.I. Sibilev*, M.A. Sibileva*: Structure of fullerene containing polivinylpyrrolidone in water solutions. *PNPI report No2238 (1998).*

K.39. V.T. Lebedev*, G.A. Evmenenko*, V.L. Alexeev*, D.M. Orlova*, Gy. Török, L. Cser, V.V.Klyubin*, A.A.Polyakov*, V.P Budtov*, P.N.Moskalev*, A.I. Sibilev*, M.A. Sibileva*: Structure of complexes of poly-N-vynilpyrrolidone with diphtalo-cyanides of rare earth elements in D_2O solutions. *PNPI report No2239 (1998)*

K.40. M.A.Kiselev*, P.Lesieur*, A.M.Kiselev*, S.Borbély, T.N.Simonova*, L.I.Barsukov*: Temperature Induced Micelle to Vesicle Transition in the DMPC/NaC system: A Small-angle Scattering Study. *Annual report of FLNP, 81-83, 1997*. JINR, Dubna, Russia.

K.41. L. Almásy, L. Cser, T. Grósz, P. Jóvári, Gy. Káli, L. Kõszegi, Gy. Mészáros, L. Rosta E. Sváb, Gy. Török: Condensed matter research. *Budapest Neutron Centre Progress Report 1993-97* (Eds.: J. Gadó, L. Rosta, I. Vidovszky) pp. 13-22 (1998)

L. INTERACTIONS OF INTENSE LASER FIELDS WITH MATTER

Gy. Farkas, S. Varró and Zs. Papp

Experiments with strong lasers on electrons in metals. — We have observed electron emission from gold cathodes irradiated by mid-IR (up to 12 microns) laser light, in the MW/cm^2 intensity range. The emission has low index of nonlinearity (close to 6, for a ratio of the work function to the photon energy close to 50), and electrons are emitted with unexpectedly wide spectrum of energies up to several eV. It is the first time that such an observation has been made under conditions which are completely free from any heating effect. Our results verify those strong field QED predictions according to which electron-electron and electron-phonon collisions change the high order coherence properties of multiphoton processes in metals.

We have demonstrated that a high energy X-ray field may be generated by shining laser light at grazing incidence on a gold target to create a surface plasma by applying, in addition, a strong static negative voltage to a metal plate parallel to the gold target at a small distance, such that the electrons are pushed back to the surface.With this arrangement powerful X-ray radiation of about 20 keV has been observed at shorter wavelengths in the ns, ps and in the femtosecond range.

Theoretical study of interaction of strong laser fields and matter. — By considering a laser-induced oscillating double layer along the surface of a metal and its action on an electron of the metal, we have shown that at moderate laser intensities of some 10^{10} W/cm^2 energetic electrons of a few 100 eV can be produced. This explains our earlier experimental results without necessarily restoring to the mechanism of Coulomb explosion, taking place after the completion of the ionization process.

We have shown that at the interface between a half space filled by laser radiation and vacuum a considerable redistribution of the energies of electrons, either scattered or ionized in the laser field, can take place. On the basis of results obtained the outcome of the experiments on photon absorption by free electrons carried out long ago in our institute can be explained.

By using the above-mentioned laser induced double layer model we were able to explain the essential features of the generation of strong X-ray pulses at metal surfaces in the presence of a static electric field.

In the framework of the QED we have treated the ponderomotive (quiver) energy conversion to final drift energy of a free electron interacting with a strong radiation field. We have shown that a large amount of energy can be transferred from the radiation field to the electron resulting in its acceleration to high energies.

Concerning quantum optics, on the basis of a new polar decomposition of the photon absorption operator we were able to define a hermitian phase operator in terms of a series convergent in norm in the whole Hilbert space of a quantized mode of the electromagnetic radiation.

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Grants

OTKA T16014 Experimental and theoretical investigation of new fundamental physical processes (laser-matter interactions) induced by laser beams of superintense (10^{15}-10^{20} W/cm^2) laser systems (Gy. Farkas, 1995-1998)

TéT F-19/97 Interaction of laser radiation with solids (Gy. Farkas, 1997-1999)

TéT A-47/97 Study of the dynamics of metallic electrons in strong laser fields (S. Varró, 1997-1998)

Publications

Articles

L.1. Gy. Farkas, Cs. Tóth, A. Kõházi-Kis, P. Agostini*, G. Petite*, P. Martin*, J.M. Berset*, J.M. Ortega*: Infrared electron photoemission from a gold surface. *J. Phys. B: At. Mol.Opt.Phys.* **B31**, L461-L468 (1998)

L.2. S. Varró, F. Ehlotzky*: High-order multiphoton ionization at metal surfaces by laser fields of moderate power. *Phys. Rev.* **A57**, 663-666 (1998)

L.3. S. Varró, F. Ehlotzky*: Redistribution of electron energies at the interface between laser-radiation-filled space and vacuum. *J. Phys. B: At.Mol.Opt.Phys.* **B31**, 2145-2151 (1998)

L.4. F. Körmendi*, Gy. Farkas : QED theory of ponderomotive energy conversion into final drift energy of the electron interacting with a laser beam. *Phys. Rev.* **A**, accepted for publication

L.5. S. Varró, F. Ehlotzky*,Gy. Farkas: Generation of X-rays by irradiating metal surfaces with a powerful laser beam in the presence of a strong static electric field. *J. Phys.* **D**: *Appl.Phys.*, accepted for publication

Others

L.6. S. Varró, F. Ehlotzky*: Redistribution of electron energies at the interface between laser-radiation-filled space and vacuum. Book of abstracts (Ed. W. Becker), *7th International Workshop on Laser Physics* (Berlin, Germany, July 6-10, 1998.) pp. 86-87.

L.7. S. Varró, Gy. Farkas: Appearance of electron and light spectra of discrete structure in the presence of superintense laser fields. Book of abstracts (Ed. G. Pásztor), *Meeting of the Roland Eötvös Physical Society* (Gödöllõ, Hungary, August 25-28, 1998.) pp. 171-172.

L.8. N. Bokor*, Zs. Papp: Study of the projection properties of holograms generated by computer. Book of abstracts (Ed. G. Pásztor), *Meeting of the Roland Eötvös Physical Society* (Gödöllõ, Hungary, August 25-28, 1998.) pp. 173-175.

M. LASER PHYSICS

M. Jánossy, G. Bánó, L. Csillag, Z. Donkó, Sz. Fórizs, Á. Hoffmann, Z. Gy. Horváth, N. Kroó, Zs. Lenkefi, P. Mezei, K. Rózsa, L. Szalai, K. Szõcs, Zs. Szentirmay

Gas laser studies. — We investigated ultraviolet and visible transitions of the cathode sputtered helium - gold laser. On the 282 nm Au-II transition 100 mW laser power was obtained in msec-long pulses. Our gain measurements showed that this transition has an exceptionally high, ≈ 50 %/m gain, significantly exceeding that measured on other transitions (e.g. 692 nm) in Au-II. The mode structure of the laser was studied on the 692 nm transition. We found that the laser operates spontaneously in a single longitudinal mode. This results from the high homogenous (collision) broadening of the spectral line due to the relatively high gas pressures (10-20 mbar).

Plasma modeling. — The cathode region of glow discharge was investigated by computer modeling. We developed a hybrid model of glow discharges which combines the fluid description of ions and slow electrons with Monte Carlo simulation of fast electrons. Our model made it possible to determine the discharge characteristics (spatial distribution of particle densities, electric field, particle fluxes) in a fully self-consistent manner. We developed a molecular dynamics simulation program to investigate the properties of one-component plasmas (strongly coupled Coulomb systems). Using a new perturbation technique we determined the transport coefficients (heat conductivity and shear viscosity) for a wide range of plasma conditions.

Electrolyte cathode atmospheric glow discharge (ELCAD). — The pressure dependence of cathodic current density was studied in case of the ELCAD using an air atmosphere, and in case of the metal cathode glow discharge operating in air and helium gas. Since, in case of the ELCAD, the plasma region above the electrolyte cathode surface is saturated by water vapour, this discharge can be considered to be such a discharge, which operates in H_2O vapour. Therefore, we can say, that our measurements were performed in three different gases, namely H_2O, N_2 and He. It is also to be noted, that for an electrolyte cathode glow discharge, the H_2O^+ molecular ions are the main particles taking part in the self-sustaining mechanism.

In all three gases, the same deviation from the similarity law $j \approx const \cdot p^2$ could be observed at and above medium pressures, which is attributed to the occurrence of the dissociative recombination of positive molecular ions. Taking into account this process, the pressure dependence of cathodic current density could be determined, from which the relation $j \approx const \cdot \sqrt{p}$ resulted. On the basis of this deduction, excluding the extreme electronegative gases, it seems that the pressure dependence of cathodic current density determined at high pressures through the dissociative recombination of positive molecular ions and given by the relation $j \approx const \cdot \sqrt{p}$, can be considered to be generally valid.

The gas temperature was calculated in the cathode surface-dark space boundary layer in the case of the ELCAD, taking into account the symmetrical charge transfer of the H_2O^+ molecular ions as a dominant collision. The gas temperature was found to be approximately 7000 K, which is in accordance with experimental results.

Determination of surface roughness parameters on randomly and periodically corrugated surfaces. — The applicability of micromechanically or laser treated

surfaces depends mostly on their surface parameters as homogenity, flatness, nano-scaled corrugations etc. Atomic force microscopy (AFM), developed in the last decade, is ideal for the experimental investigation of surface roughness. Our principal aim was to compare the roughness parameters obtained by AFM and with a conventional optical method on natural and artificially roughened gold films.

The quality of a thin metal layer is characterized by its optical parameters, e.g. the complex dielectric function which can be determined by normal reflectometry, ellipsometry, and if the metal allows surface plasmons by attenuated total reflection (ATR) spectrometry. However, since the natural surface roughness of the substrate and of the layer may drastically influence the measured optical parameters, information on surface roughness is of primary importance for the preparation of any kind of thin film device. In order to study the effect of surface roughness on the optical properties of gold films, we performed ATR measurements on samples whose LiF sublayers were of different thickness, obeying different roughness structures.

Research on multidimensional lasers. — The role of internal plasma mirror shells appearing in a natural way in all gravitationally confined dense plasmas of stars because of the fundamental optical properties of plasmas has been investigated theoretically. It was found that the effect of color sensitive, geometrically seperated reflecting shells results in a more abrupt limb darkening for light of shorter wavelength than that of longer ones along the diameter of observed disc of stars. The solar photosphere strongly screens the phenomena in the nearest star, but the natural existence of "mirrors" in cosmic objects is expected to strongly influence the spatial light distribution of the recently discovered multidimensional "laser-stars".

Photodynamic therapy. —In the field of photodynamic therapy of bacterial cells a significant killing of *Escherichia coli B.* cells under white light irradiation was realised. Prior to the photoinactivation measurements the optimal conditions were determined for photodynamic inactivation of the *E. coli B.* cells. On the basis of fluorescence emission spectra and introducing a simple statistical method the concentration of fluorophors in solutions was determined.

Neural system for real-time evaluation of spectra. — A laboratory model was realized to demonstrate the possibilities of neural network data handling of optical information. Concrete applications of the experimental setup for medical and drug analysis are in progress.

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Grants:

OTKA T-14909 Lasers in high-efficiency hollow cathode discharges (K. Rózsa, 1995-1998)
OTKA F-15502 Basic processes of glow discharge in the cathode region (Z. Donkó, 1995-1998)
OTKA T-25941 Ultraviolet lasers in controllable-temperature hollow cathode discharge (K. Rózsa, 1998-2001)
OTKA T-25989 Numerical modelling of gas discharge plasmas (Z. Donkó, 1998-2001)
OTKA F-25503 Hollow cathode discharges and lasers in gold vapor (L. Szalai, 1998-2001)
OTKA T-017293 Multidimensional lasers (Z. Gy Horváth; 1996-1998)
OTKA T-014850 Electrolyte cathode atmospheric glow discharge (P. Mezei, 1995-1998)
OTKA T-016075 Electromagnetic modes of metal/dielectric interfaces (N. Kroó, 1995-1998)
OTKA T-020089 Optical parameters of fulleren films (Zs. Szentirmay, 1996-1999)
OTKA T-022074 Investigation of metal fulleren films with laser reflectometry (Á. Hoffmann, 1997-2000)

Publications

Articles

M.1. Z. Donkó, L. Szalai, K. Rózsa, M. Ulbel*, M. Pöckl*: High gain ultraviolet Cu-II laser in a segmented hollow cathode discharge. *IEEE J. Quantum Electronic*s **34**, 47-53 (1998).

M.2. Z. Donkó: Hybrid model of a rectangular hollow cathode discharge. *Phys. Rev.* **E57**, 7126-7137 (1998).

M.3. Z. Donkó, K. Rózsa, L. Szalai: High voltage hollow cathode discharges: Laser applications and simulations of electron motion. *Plasma Physics Reports* **24**, 588-598 (1998).

M.4. Z. Donkó, B. Nyiri*, L. Szalai, S. Holló*: Thermal conductivity of the classical electron one component plasma. *Phys. Rev. Lett.* **81,** 1622-1625 (1998).

M.5. P.Mezei, T.Cserfalvi*, M.Jánossy: The gas temperature in the cathode surface-dark space boundary layer of an electrolyte cathode atmospheric glow discharge (ELCAD). *J. Phys. D: Appl. Phys*. **31,** L41-L42 (1998).

M.6. P.Mezei, T.Cserfalvi*, M.Jánossy, K.Szõcs and H.J.Kim*: Similarity laws for glow discharges with cathodes of metal and an electrolyte. *J. Phys. D: Appl. Phys.* **31,** 2818-2828 (1998).

M.7. A. Hoffmann, Z. Lenkefi, Z. Szentirmay: Effect of roughness on surface plasmon scattering in gold films. *J. Phys.: Condens. Matter* **10**, 5503-5513 (1998).

M.8. M. Jánossy, P.Mezei: Excitation of the 210 nm Zn-II line in a He-Ne-Zn hollow cathode discharge. *Zeitschrift für Naturforschnung A.*, accepted for publication

Conference proceedings

M.9. Z. Donkó: Hybrid modeling of self-generated oscillations in a hollow cathode discharge. In: *Proc. of 11th Symp. on Elementary Processes and Chemical Reactions in Low Temperature Plasma,* Liptovsky Ján, Slovakia, Eds: M. Morvová and K. Hensel, 1998, Contributed papers, Part 1, pp. 54-57.

M.10. T. M. Adamowicz*, G. Bánó, L. Szalai, K. Dzieciolowski*, W. Kwasniewski*, Z. Donkó, K. Rózsa: High gain cathode sputtered He-Zn laser in a segmented hollow cathode discharge. In: *Proc. of 11th Symp. on Elementary Processes and Chemical Reactions in Low Temperature Plasma,* Liptovsky Ján, Slovakia, Eds: M. Morvová and K. Hensel, 1998, Contributed papers, Part 1, pp. 11-14.

M.11. L. Szalai, T. M. Adamowicz*, A. M. Tokarz*, G. Bánó, K. Kutasi, Z. Donkó, K. Rózsa: Operation characteristics of a segmented hollow cathode Au ion laser. In: *Proc*. of *11th Symp. on Elementary Processes and Chemical Reactions in Low Temperature Plasma,* Liptovsky Ján, Slovakia, Eds: M. Morvová and K. Hensel, 1998, Contributed papers, Part 1, pp. 157-160.

M.12. L. Szalai, T. M. Adamowicz*, A. M. Tokarz*, G. Bánó, K. Kutasi, Z. Donkó, K. Rózsa: Optimum operating conditions of a hollow cathode Au-II laser. In: *Proc. of SPIE, 3573, Optika'98: 5th Congress on Modern Optics*, Budapest, Hungary, Eds: Gy. Ákos, G. Lupkovics and A. Podmaniczky, 1998, pp. 28-31.

M.13. T. Cserfalvi*, P. Mezei, H. J. Kim*: Analytical applications of the electrolyte cathode atmospheric glow discharge. In: *Proc. of the 25th annual meeting of FACSS*, Austin, Texas, USA, October 11 - 16, 1998.

M.14. Z. Szentirmay, A. Hoffmann, N. Kroo, Z. Lenkefi: Determination of surface roughness parameters on randomly and periodically corrugated surfaces. In: *Proc*. of *10th Seminar on Precision Machining: Laser Beam Micromachining, Budapest, Hungary, 1998.*

M.15. A. Hoffmann, N. Kroó, Z. Lenkefi, Z. Szentirmay: Multiwavelength ATR reflectometry of thin films. In: *Proc. of SPIE, 3407, International Conference on Applied Optical Metrology, Budapest, Balatonfüred, Hungary,* Eds: P. K. Rastogi, F. Gyimesi, 1998, pp. 256-261.

M.16. Sz. Fórizs, Z. Gy. Horváth, T. Lohner*, M. Fried*, I. Bársony*: PC controlled CCD matrix based optical multichannel analyser for "RESPECT" measurements. In: *Proc. of SPIE, 3573, Optika'98: 5th Congress on Modern*

Optics, Budapest, Hungary, Eds: Gy. Ákos, G. Lupkovics and A. Podmaniczky, 1998, pp. 230-231.

M.17. T. Lohner*, M. Fried*, E. Vázsonyi*, P. Petrik*, L. Rédei*, I. Bársony*, Sz. Fórizs, Z. Gy. Horváth : Optical characterization of as-prepared and oxidized porous silicon layer structures. In: *Proc. of SPIE, 3573, Optika'98: 5th Congress on Modern Optics, Budapest, Hungary*, Eds: Gy. Ákos, G. Lupkovics and A. Podmaniczky, 1998, pp. 118-119.

M.18. L. Rédei*, M. Fried*, T. Lohner*, O. Polgár*, I. Bársony*, Sz. Fórizs, Z. G. Horváth, J. Humlicek*, H. Wallinga*: Concept of neural system for real-time evaluation of spectroscopic measurements. In: *Proc. of SPIE, 3573, Optika'98: 5th Congress on Modern Optics, Budapest, Hungary*, Eds: Gy. Ákos, G. Lupkovics and A. Podmaniczky, 1998, pp. 155-159.

Book chapter

M.19. P. Apai, P.Mezei: Gázlézerek erõsítésének és longitudinális módusainak vizsgálata (Investigations of the longitudinal modes and the gain of gas lasers, in Hungarian). In: *Introduction into modern optics*. Vol. IV. Műegyetemi Kiadó, Bp. 1998. J 050-394.

Others

M.20. L. Szalai, G. Bánó, K. Kutasi, Z. Donkó, K. Rózsa: Optimization of hollow-cathode discharges for pumping metal ion lasers. In: Book of abstracts of *Tenth International School on Quantum Electronics, Lasers - Physics and Applications*, Varna, Bulgaria, 1998, p.11.

M.21. Z. Donkó, B. Nyíri*, L. Szalai, S. Holló*: Transport coefficients of the classical one-component plasma from nonequilibrium molecular dynamics simulations. *APS Division of Plasma Physics, Annual Meeting,* New Orleans, 16-20 Nov. 1998 (abstract)

M.22. Z. Horváth, Z. Donkó: Lehetséges fizikai magyarázat az alacsony energiájú lézeres biostimulációs hatásra (A Possible Physical Explanation of Low Power Laser Biostimulation Effect, in Hungarian). In: *4th National Medical Laser Congress*, Budapest 1998. (abstract)

M.23. Z. Horváth: Nem mind lézer, ami fénylik (Not all is laser which shines, in Hungarian). In: *4th National Medical Laser Congress,* Budapest 1998. (abstract)

M.24. Sz. Fórizs, Z. G. Horváth: Kábítószer kimutatása reagens nélküli optikai spektroszkópiával (Drog detection without reagents by optical spectroscopy, in Hungarian). In: *4th National Medical Laser Congress,* Budapest 1998. (abstract)

M.25. K. Szőcs: Az élet fényei a biológiai diagnosztikában (Life`s light in biological diagnostics, in Hungarian). In: *4th National Medical Laser Congress,* Budapest 1998. (abstract)

M.26. K. Szőcs, F. Gábor*, G. Csik*, J. Fidy*: Endogenous Porphyrin accumulation by Escherichia Coli B. *7th Biennal Congress, International Photodynamic Association*, Nantes, France 1998.

N. LASER APPLICATIONS

I. Kertész, P. Apai, A. Czitrovszky, P. Jani, Á. Kiss, M. Koós, S. Lakó, Gy. Messing, Said H. S. Mustafa, A. Nagy, B. Plósz, I. Pócsik

Solid state laser development. — A high average power Nd:YAG laser was applied for welding of aluminium at the Technical University Stuttgart using our piezo-drivan Fabry-Perot Q-switch. Our expectation was that the Q-switched mode is not adequate to welding but the results are promising.

Luminescent properties of Gd^{3+} have been studied using multistage up-conversion excitation of Yb-Tm-Gd doped material. InGaAs laser diode was used for pumping and UV luminescence of Gd was observed in the 204-312 nm range. This proves that the Gd^{3+} ion really can be considered as a potential laser ion for UV lasers.

Optical measurement technique. — Experimental equipment for generation of entangled two-photon field was developed. The improvement of the parameters of the system was achieved by using of constant fraction discriminators and a new data evaluation. The rate of photon detection coincidence for entangled photon pairs was measured with 50ps time window.

The optic end electronic system was elaborated for standardless measurement of quantum efficiency of avalanche photodiodes using two-photon field.

Experimental equipment was developed for the measurement of single-photon and two-photon peaks in the photomultipliers for photon counting.

Experiments were carried out and software package was developed for the simultaneous measurement of velocity and size of nanometer size aerosol particles.

Dispersity, structure, composition and concentration of aerosol particles released from simulant fuel rods was studied.

The measurement of size distribution of high temperature aerosols released from fuel rods in the frame of EU CODEX AIT experiment was performed. The concentration of nuclear aerosols was measured within 10^5 dynamic range at various stages of the heating up to 2200 ^{o}C. The peaks of concentration corresponding to the preoxidation and oxidation period were recorded using two airborne particle counters in different sampling points of the facility. The evaluation of the results was made using different database programs.

Amorphous thin layers. — Our research work in this year was oriented towards the investigations of amorphous carbon (a-C:H) and one of its component, the graphitic structures. The structural and macroscopic properties related to localized states in the gap and near the band edges of amorphous carbon thin films were studied by several methods.

The Raman investigations proved, that both characteristic Raman bands of graphite originates from the same E_{2g2} basic vibration mode of the graphite single crystal. The G band corresponds to the normal zone-centre Raman process, where the momentum transfer is small. The D band is an electron excitation enhanced resonance Raman process, which shows a strong dispersion. We have explained this dispersion by the combined electron energy dispersion and phonon dispersion. According to the energy of the exciting laser electron excitation takes place, and a phonon, with exactly the same momentum is emitted, which phonon generates the Raman shift of the scattered

photons. The available laser energies are in the zone-boundary region of the Brillouin zone of the graphite crystal. This gives the birth of a new structure investigating method, where the Raman scattering supplies information about the high momentum regions of the Brillouin zone as well, which was previously investigated by neutron scattering only.

Influence of nitrogen doping on photoluminescence properties of a-C:H layers was demonstrated by studying sample series with different N concentrations. Small N concentration quenches the light emission of a-C:H layers completely. By increasing the N concentration new light emission appears in different energy range. This band depends slightly on N concentration.

Spectral ellipsometry was applied to determine the optical constants of a-C:H layers in the photon energy range of 1.5-4.5 eV. The a-C:H layers were deposited onto silicon wafers by our decomposition method of methane in a radio frequency (rf) glow discharge process. Series of thin films were prepared by varying the negative self bias ($U_{S.b.}$) in the range of -600 V < $U_{S.b.}$ < -200 V. The a-C:H samples in this series exhibit transition in electrical and optical properties with decreasing optical gap from 1.3 eV to 0.7 eV as the deposition voltage changes in the range of 200 - 600 V. The complex dielectric function [$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$] and the complex refractive index [$N(\omega) = n(\omega) + ik\omega$)] were determined for the samples. The most pronounced changes in optical constants and in bonding structure occur near -500 V self bias. The $\varepsilon_2(\omega)$spectrum exhibits a broad maximum which shifts to lower energies by increasing deposition self bias. The optical properties were explained in terms of electronic band structure related to sp^3 and sp^2 hybridised bonding states of carbon atoms and to intermediate range ordering of sp^2 bonded sites.

In a co-operation we started to investigate the a-C:H film surfaces with atomic force microscope (AFM). Beside the precisely flat surface of the film we have found some hemi-spherical structures, which seems to resist the intensive ion-implantation process of the film formation, and seems to have a stronger growth tendency, than the film itself. These are preliminary results, which will be continuing, but the strongly increasing interest towards the new carbon formations make it worth to investigate in more details.

Grants

OTKA 20202 Development of fundamental experiments with squeezed light (A. Czitrovszky, 1996-1999)

OTKA T025707 Investigation of nano structures of composit metal-ceramic structures appliing interferometric methods (P. Jani, 1998 – 1999)

OMFB 97-97-47-1593, Integrated optical sensor for the measurement of dynamic properties of aerosol particles (P. Jani, 1997-1999)

OMFB-Technoorg-SZFKI 97-97-47-1592, Investigation of nuclear aerosols (A. Czitrovszky, 1998-1999)

AKP 96/2-615 2.2 Development of high time resolution and high quantum efficiency photodetection system (A. Czitrovszky, 1997-1998)

OTKA T-026073 Electronic states, charge carrier localization and their interaction with the structure in amorphous carbon films (M. Koós, 1998-2000)

OTKA T-025540 STM/AFM investigations of atomic and mesoscopic structures of amorphous carbon (I. Pócsik, 1998-2000)

Publications

Articles

N.1. N. V. Baburin*, Yu. V. Borozdov*, Yu. K. Danileiko*, B.I. Denker*, A. D. Ivanov*, R. Ifflander*, I. Kertész, N. Kroó, V. V. Osiko*, S. E. Sverchkov*, A. V. Sidorin*, R. Hack*, V. A. Chikov*: Q-switching of a high-power solid-state laser by a fast scanning Fabry-Perot interferometer. *Quantum Electronics (RU)* **25,** 633-637 (1988)

N.2. A. Czitrovszky, P. Jani, L. Maróti*, L. Matus*, P. Windberg*: Composition and concentration of aerosol particles released from simulant LWR fuel rods. *Journal of Aerosol Science* **29S1**, 471-472 (1998).

N.3. A. Czitrovszky, P. Jani, L. Maróti*, L. Matus*, A Pintér*, P. Windberg*: Dispersity and structure of aerosol particles released from simulant LWR fuel rods. *Journal of Aerosol Science* **29S1**, 469-470 (1998)

N.4. P. Jani, A. Nagy, A. Czitrovszky: Single nanoparticle size measurement algorithm using photon correlation techniques. *Journal of Aerosol Science* **29S1,** 419-420 (1998)

N.5. M. Koós, I. Pócsik, J. Erostyák* and A. Buzádi*: Amorphous Carbon Luminescence: Excitation and Emission in a Broad Energy Range. *Journal of Non-Crystalline Solids* **227-230**, 579-582 (1998).

N.6. I. Pócsik, M. Hundhausen*, M. Koós and L. Ley*: Origin of the D peak in the Raman Spectrum of Microscystallline Graphite. *Journal of Non-Crystalline Solids* **227-230,** 1083-1086 (1998).

N.7. S.H. Moustafa, M. Koós and I. Pócsik: DC Electric Properties of Amorphous Carbon with Different Bonding Hybridization. *Journal of Non-Crystalline Solids* **227-230**, 1087-1091 (1998).

N.8. R. Blinc*, D. Arcon*, P. Cevc*, I. Pócsik, M Koós, Z. Trontelj* and Z. Jaglicic*: ^{13}C Magnetic Resonance and Electron Spin Resonance of Amorphous Hydrogenated Carbon. *Journal of Physics; Condensed Matter* **10**, 6813-6824 (1998).

N.9. D. Arcon*, J. Seliger*, R. Blinc*, I. Pócsik and M Koós: ^{13}C and ^{1}H Spin-Lattice Relaxation in Amorphous Hydrogenated Carbon. *Solid State Communication* **107**, 349-352 (1998).

Conference proceedings

N.10. M. Koós, T. Lohner*, S.H. Moustafa and I. Pócsik: Optical Properties of Hydrogenated Amorphous Carbon Determined by Spectral Ellipsometry. In: *Proc. of "Optika '98" 5th Congress on Modern Optics, Budapest, 14-17 Sept. 1998,* SPIE **3573**, 1998, pp. 328-331.

N.11. B. I. Denker*, B. I. Galagan*, V. V. Osiko*, S. E. Sverchkov*, I. Kertész: UV luminescence in $Y6^{3+}$-Tm^{3+}-Gd^{3+} system excited by IR laser diode. In: *Proc. Conf. OSA TOPS 19. Advanced Solid State Lasers,* eds. Rosemberg and Fejer, Opt. Soc. Am., 1998, pp. 450-453.

N.12. A.Czitrovszky, A. Nagy, T. Mosoni*, P. Jani, K. Bodnár*, Á. Illés: A new sizing method for liquid-borne particles with high dynamic range. In: *Proc. of "Optika '98" 5th Congress on Modern Optics, Budapest, 14-17 Sept. 1998,* SPIE **3573**, 1998, pp. 225-229.

N.13. A.Czitrovszky, A. Sergieenko*: Mesurement of qantum efficiency of avalanche photodetectors based on quantum two-photon field. In: *Proc. of "Optika '98" 5th Congress on Modern Optics, Budapest, 14-17 Sept. 1998,* SPIE **3573,** 1998, pp. 332-334.

N.14. A.Czitrovszky, A. Nagy, P. Jani: Estimating of the shape factor of suspended particles in a liquid-borne particle counter. In: *Proc. of Internat. Conf. on Applied Optical Metrology, Balatonfüred, Hungary 1998,* Eds: P.K. Rastogi, F. Gyimesi, SPIE **3407,** 1998, pp. 250-255.

N.15. P. Jani, A. Nagy, A. Czitrovszky: Size distribution of particles in LDA system using back scattering geometry. In: *Proc. of Internat. Conf. on Applied Optical Metrology, Balatonfüred, Hungary 1998,* Eds: P.K. Rastogi, F. Gyimesi, SPIE **3407,** 1998, pp. 262-266.

N.16. I. Pócsik, M. Hundhausen*, M. Koós, O. Berkesi* and L. Ley*: Resonance Raman phenomena in Raman spectroscopy of graphite. In: *Proceedings of the Sixteenth International Conference on Raman Spectroscopy* Edited by A.M. Heyns, John Wiley and Sons, New York 1998. Suppl. Vol. pp.: 64-65.

N.17. I. Pócsik, M. Koós, O. Berkesi* and M. Hundhausen*: Advantage of infrared excitation in Raman spectroscopy of hydrogenated amorphous carbon films. In: *Proceedings of the Sixteenth International Conference on Raman Spectroscopy.* Edited by A.M. Heyns, John Wiley and Sons, New York 1998. Suppl. Vol. pp.: 66-67.

N.18. I. Pócsik, M. Hundhausen*, M. Koós, O. Berkesi* and L. Ley*: Resonance Raman phenomena in Raman spectroscopy of graphite. In: *Proceedings of the International Symposium on Carbon; Science and Technology for New Carbons.* Carbon Society of Japan, Tokyo 1998. pp.: 652-653.

N.19. I. Pócsik and M. Koós: Cooling rate dependence on T_g, - caused by clustering. In: *APS Conference Proceedings* (accepted for publication)

N.20. I. Kertész, B. Plósz, Yu. K. Danilejko*, B. I. Denker*: Q-switching of high average power Nd:YAG laser for material processing. In: *Proc. Hungarian-South Korean Conference on Lasers*, Budapest, 1998 (accepted for publication)

Book chapters

N.21. I. Pócsik, M. Koós, M. Hundhausen* and L. Ley*: Excitation energy dependent Raman and photoluminescence spectra of hydrogenated amorphous carbon. In: *Amorphous Carbon: State of Art,* Ed. by S.R.S. Silva, J. Robertson, G.A.J. Amaratunga and W. I. Milne, Word Scientific, Singapore 1998. pp. 224-233.

N.22. M. Koós and I. Pócsik: Luminescence properties of hydrogenated amorphous carbon. In: *Actual problems in luminescence research*, Eds. N. Marek and K. Szabo, Pécs, 1998, pp. 281-304.

O. OPTICAL THIN FILMS

K. Ferencz, R. Szipõcs

Optical thin film structures in femtosecond laser systems. — Continuing our research started in 1993, dispersive dielectric mirrors were developed for different femtosecond laser systems such as low-loss chirped mirrors for mode-locked Cr:LiSGaF, Cr:LiSAF lasers, broadly tunable cw and modelocked Ti:sapphire lasers, as well as IR KTP based parametric oscillators and high power femtosecond amplifiers. Special ultrabroadband chirped mirrors have been developed for pulse compression experiments at the University of Groningen, the Netherlands and at the Technical University of Vienna, Austria. The pulse duration of the compressed pulses is below 5 fs at both laboratories. Using the high power compressed pulses of the commonly developed Ti:sapphire amplifier system built at the TU Vienna, coherent X-ray emission was detected from a laser induced He plasma in the water window. The aim of the present development is generation of X-ray radiation having higher power, which makes it possible for practical applications such as X-ray microscopy and microlithography. Special X-ray filter sets was developed for these applications.

Other developments on optical coatings. — Low loss dielectric mirrors have been developed for hollow cathode copper and gold lasers. The mirrors have been successfully tested at the Department of Laser Physics. Our work on optical waveguides deposited on optical gratings are still in progress for optical sensors used for medical applications. We investigated the effect of surface relief grating on the morphology and waveguiding properties of the deposited dielectric layers. Transparent electrodes were developed for porous silicon light emitters.

Publications

Articles

O.1. G. Tempea*, F. Krausz*, Ch. Spielmann*, K. Ferencz: Dispersion control over 150 THz with chirped dielectric mirrors. *IEEE Journal of Selected Topics in Quantum Electronics* **4**, 193-196 (1998)

O.2. M. Schnürer*, Ch. Spielmann*, P. Wobrauschek*, C. Streli*, N.H. Burnett*, C. Kan*, K. Ferencz, R.Koppitsch*, Z. Cheng*, T. Brabec*, F. Krausz*: Coherent 0.5-keV X-ray emission from helium driven by a sub-10-fs laser. *Phys. Rev. Lett.* **80**, 3236-3239 (1998)

O.3. L. Xu*, G. Tempea*, Ch. Spielmann*, F. Krausz*, A. Stingl*, K. Ferencz, S. Takano*: Continuous-wave mode-locked Ti:sapphire laser focusable to 5×10^{13} W/cm^2. *Optics Letters*. **23,** 789-791 (1998)

P. GROWTH AND CHARACTERIZATION OF OPTICAL CRYSTALS

I. Földvári, L. Bencs, E. Beregi, V. Horváth, Á. Péter, K. Polgár, O. Szakács, Z. Szaller

Growth and study of nonlinear borate crystals. — The cyclic borates exhibit excellent nonlinear optical (NLO) properties and wide transparency range down to the vacuum ultraviolet. Single crystals of β-barium metaborate - **BaB_2O_4 (BBO)** were grown by the top-seeded high temperature solution (flux) method. The quality of BBO crystals were tested by optical microscopy and chemical etching. The polarization dependence of the Raman spectra of BBO crystals was measured and analyzed. All the predicted external and internal vibration modes were observed and assigned. A correspondence between the lattice and free-ring modes was presented.

The huntite type double borates, $RM_3(BO_3)_4$ (where R^{3+} = Sc, Y, La, Lu, In, Bi and M^{3+} = Al, Cr, Ga, Fe, Sc), have good NLO parameters and these crystals can easily be doped with rear earths (e.g. Nd, Ga, Er) and transition metals (e.g. Cr) for building microchip lasers. Spontaneous nucleation and top-seeded flux methods were developed to grow **yttrium-aluminum borate -- $YAl_3(BO_3)_4$ (YAB)** single crystals. Undoped, Nd, Er and Cr doped YAB crystals were grown. Differences were shown in the lattice parameters and the morphological formations among the various doped crystals. The composition, structure and quality of the YAB crystals were tested by X-ray diffraction, energy dispersive X-ray spectrometry, scanning electron microscopy and Fourier Transformation Infrared Absorption Spectroscopy.

Growth and study of bismuth oxide based crystals. — Bismuth tellurite - Bi_2TeO_5 is a novel nonlinear crystal with interesting physical parameters. The crystal structure contains 18 % open oxygen positions and the coordination varies between 5 and 8 around the different cation sites. The material, therefore, is an excellent host for several dopants with segregation coefficients close to unity. The most interesting feature of the crystal is a long living (years) photorefractive signal that developed in the four wave mixing process without specific fixing.

Single crystals of pure and doped Bi_2TeO_5 were grown by the Czochralski technique. The specific method developed in our laboratory solved the problem of TeO_2 evaporation from the melt and the related compositional changes. This was the first published growth of optical quality Bi_2TeO_5 crystals.

Strong photochromic effect was observed in the Cr-doped Bi_2TeO_5 crystals. There was a single absorption band in the as grown crystal peaking at 434 nm (77 K data). This band belonged to Cr^{6+} ions in a perturbed octahedral ligand field at Te lattice sites, capturing an extra oxygen (chromate anion). The photochromic effect is related to Cr^{6+} — Cr^{5+} transition and resulted in a complex absorption spectrum in the visible and near infrared region. The fine structure of the Cr^{5+} ligand field spectra allowed us to determine the local symmetry of the Cr ions (D_{2d}). The temperature dependence of the Cr^{5+} production indicated that there was a thermally activated step in the photochromic process. The photochromic effect could entirely be reverted by thermal annealing (250 °C).

The polarized Raman spectra of Bi_2TeO_5 crystals were determined and analyzed. The temperature dependence of the spectra was followed in the 10 - 890 K range. No

specific changes were observed that might be related to second order phase transition. It was shown that the 762 cm^{-1} Raman line was very sensitive to detect the oxidation status of the crystals. The oxidation of the Bi_2TeO_5 structure to Bi_2TeO_6 begins above 500 °C and the process is complete at about 600 °C. The release of the captured oxygen is very slow at room temperature. Since during growth the crystal passes through the temperature range where Bi_2TeO_6 is stable, such a non-destructive test as to measure the intensity of the 762 cm^{-1} Raman line to detect the actual oxygen status is rather important.

A complex X-ray power diffraction (XPD), selected area electron diffraction (SAED) and differential scanning calorimetric analysis was applied to determine the phase transitions of another bismuth oxide - tellurium oxide compound, $Bi_2Te_4O_{11}$. A metastable cubic and a monoclinic ($P2_1/n$) final structure were identified. A unique multi-step transfer was observed from the cubic to the monoclinic phase. The first step was the re-arranging of the cations. The intermediary product was a mixture of rutile type TeO_2 and fluorite based $Bi_2Te_2O_7$. The ordering of the oxygen sublattice was a separable final phase to generate the monoclinic $Bi_2Te_4O_{11}$. The oxygen deficient structures of the $Bi_2Te_4O_{11}$ phases made this kinetic possible.

Growth and study of stoichiometric lithium niobate. — Lithium niobate $LiNbO_3$ is one of the most widely used nonlinear crystals. The melt grown crystals of $LiNbO_3$ show typical non-stochiometric character that can be described by excess Nb ions in Li sites (antisite Nb). This kind of defect structure reduces some important physical parameters of the crystals and, consequently, it limits their applicability. There is a worldwide effort to produce stoichiometric $LiNbO_3$ crystals.

Stoichimetric $LiNbO_3$ crystals were grown by a top-seeded flux method developed in our laboratory. The composition and quality of the crystals were analyzed by the absorption edge position method developed also in our laboratory. The widest observed transparency range and a recent tests by nuclear methods (Perturbed Angular Correlation and Ion Beam Channeling) showed that this technique has resulted in the crystal composition closest to the given formula. The dependence of the $\mathbf{r}_{61}$ electro optic (EO) coefficient was determined as a function of the crystal composition. The non-monotone change in $\mathbf{r}_{61}$ related mainly to the electro-mechanical contribution. The enhanced EO properties and the increased resistance to optical damages make the stoichiometric crystals attractive for laser applications.

A key question for the application of doped $LiNbO_3$ crystals is the actual lattice sites of the dopants. Single and double doped congruent $LiNbO_3$ crystals were grown by the Czochralski technique. It was shown that both the crystal composition and selected co-dopants (e.g. Mg) modify the incorporation and physical characteristics of active dopants.

Analytical spectroscopic investigation of oxide crystals. — The matrix effect of the host material is a major factor in the atomic absorption spectroscopic (AAS) analysis of the dopant in crystals. The stabilizer containing solvent technique developed for transition metals in Bi_2TeO_5 was compared with solvent and direct analysis by ICP (plasma spectroscopy). The sensitivity and reproducibility of our AAS method was shown to be competitive to the ICP and the data obtained with the two methods were the same within the error limit.

The following other crystals were grown for research and development studies that are not discussed above: lithium triborate - **LiB_3O_5 (LBO),** lithium tetraborate - **$Li_2B_4O_7$**

(LTB), cesium-lithium borate -- **$CsLiB_6O_{10}$ (CLBO),** paratellurite -- **TeO_2,** sillenites -- **$Bi_{12}GeO_{20}$, $Bi_{12}TiO_{20}$ and $Bi_{12}SiO_{20}$,** zinc tungstate -- **$ZnWO_4$** and germano-eulytine -- **$Bi_4Ge_3O_{12}$**.

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Grants

OTKA T 014884	Growth and study of bismuth oxide based photorefractive materials (I. Földvári, 1995-98)
OTKA T 024091	Growth and study of nonlinear optical crystals transparent in the far UV region (K. Polgár, 1997-2000)
OTKA T 023737	Developing and applying spectroscopic methods for analyzing the dopants and trace elements in bismuth oxide based crystals (O. Szakács, 1997-99)
OTKA T 026647	Study of solid phase reactions for growth of nonlinear optical crystals (L. Pöppl (ELTE) and I. Földvári, 1998-2000)
HAS - CONACYT (Mexico) joint project:	Growth, linear and nonlinear spectroscopy of new potential laser crystals (I. Földvári, 1998-2000)
HAS - Armenian Academy joint project:	Growth and study of nonlinear optical crystals. (K. Polgár, 1996-2000)
COST Action P2	Application of nonlinear optical phenomena: Project WG1/1. Materials and systems for optical data storage (I. Földvári, 1998-2001) Project WG2/4. Nonlinear optics for quantum communication (K. Polgár, 1998-2001) Project WG3/7. Optical synthetizers (I. Földvári, 1998-2001)

Publications:

Articles:

P.1. I. Földvári, L.A. Kappers*, R.H. Bartram*, R. Capelletti*, Á. Péter: Photochromic effects in Bi_2TeO_5:Cr crystals. *Opt. Mater.* **10,** 47-53 (1998)

P.2. R.S. Klein*, W. Fortin*, I. Földvári and G.E. Kugel*: Raman spectra in Bi_2TeO_5 as a function of the temperature and the polarization. *J. Phys. Condens. Mater.* **10,** 3659-68 (1998)

P.3. P. Ney*, M.D. Fontana*, A. Maillard*, K. Polgár: Assignment of Raman lines in β-BaB_2O_4 single crystals. *J. Phys Cond Matter,* **10**, 673-681 (1998).

P.4. L.G. Rakitina*, B.D.Shanina*, G.Corradi, K.Polgár: Electron transfer through ordered metallic chains in $LiNbO_3$(Mg;Zn):Me $3d^1$. *J. Magnetism and Magn. Mater.* **184**, 238-240, (1998) (see also: Q.9.).

P.5. F. Abdi*, M. Aillerie*, P. Bourson*, M.D. Fontana*, K. Polgár: Electro-optic properties in pure $LiNbO_3$ crystals from the congruent to the stoichiometric composition. *J. Appl. Phys.* **84**, 2251-54, (1998)

P.6. G. Corradi, I.M. Zaritskii*. A. Hofsaetter*, K. Polgár, L.G. Rakitina*: Ti^{3+} on Nb site - A paramagnetic Jahn-Teller center in vacuum-reduced $LiNbO_3$:Mg,Ti single crystals. *Phys. Rev.* B. **58,** 8329-37 (1998) (See also Q.8.).

P.7. Gy. A. Lovas*, I. Dódony*, L. Pöppl* and Zs. Szaller: On the phase transition of $B_2Te_4O_{11}$. *J. Solid State. Chem.* **135**, 175-81 (1998)

P.8. L. Bencs, K. Raksányi, O. Szakács, L. Kovács, A. Watterich and Á. Péter: Removal of iron, chromium and sodium impurities from zinc tungstate ($ZnWO_4$), *J. Crystal Growth,* **181**, 455-458 (1997) (See also Q.3.).

P.9. I. Földvári, Á. Péter, O. Szakács, A. Munoz F*.: Improvement in quality and performance of photorefractive Bi_2TeO_5. *J. Cryst. Growth* 1998, accepted for publication

P.10. I. Földvári, R.S. Klein*, G.E. Kugel* and Á. Péter: Oxygen equilibrium and its detection in Bi_2TeO_5 crystals by Raman spectroscopy. *Rad. Eff. Def. in Sol.* 1998, accepted for publication

P.11. I. Földvári, A. Munoz F*., E. Camarillo*, Á. Péter and O. Szakács: Basic spectroscopic properties of Bi_2TeO_5:Er single crystals. *Rad. Eff. Def. in Sol.* 1998, accepted for publication

P.12. L.A. Kappers*, O.R. Gilliam*, R.H. Bartram*, I. Földvári and A. Watterich: A study of optical and ESR radiation-induced absorptions in TeO_2 single crystals. *Rad. Eff. Def. in Sol.* 1998, accepted for publication (see also Q.11.)

P.13. J.G. Marques*, A Kling*, J.C. Soares*, M.F. da Silva*, R. Vianden*, K. Polgár, E. Diéguez*, F. Agulló-López*, Structural defects in congruent and near stoichiometric $LiNbO_3$. *Rad. Eff. Def. in Sol.*, accepted for publication

P.14. E. Beregi, E. Hartmann, L. Malicskó and J. Madarász*: Growth and Morphology of Nd3+, Er^{3+} and Cr^{3+} doped $YAl_3(BO_3)_4$ Single Crystals. *Crys. Res. Techn.* 1998, accepted for publication (see also Q.10.)

P.15. R. Capelletti*, I. Földvári, Á. Péter and L. Seravali*: The OH vibrational spectrum in Bi_2TeO_5 single crystals. *Rad. Eff. Def. in Sol.* 1998, accepted for publication

P.16. L. Grigorjeva*, D. Millers*, G. Corradi, K. Polgár and V. Pankratov*: Induced optical absorption and relaxation process in $LiNbO_3$. *Rad. Eff. Def. in Sol.*, accepted for publication (see also Q.15.).

Conference procceding

P.17. L. Kovács, E. Beregi, K. Polgár and Á. Péter: FTIR Spectroscopy of Borate Crystals. In: *Proceedings of International Conference on Solid State Crystals, 12-16 October, 1998, Zakopane, Poland*, SPIE, accepted for publication (see also Q.17.)

Book chapter

P.18. Földvári I. and Péter Á.: Kristályoptika, Bevezetés a modern optikába, szerk. Richter P. 4. fej. Egyetemi jegyzet, Müegyetemi Kiadó, Budapest, 1998. (Chapter 4. Crystal Optics. In: P. Richter, ed. Introduction to modern optics, University textbook, Technical University, Budapest, 1998, in Hungarian)

Others:

P.19. E. Beregi, V. Izvekov*, L. Kovács, Á. Péter and K. Polgár: FTIR spektroszkópiai vizsgálatok borát kristályokon. (FTIR spectroscopic Investigation of borate crystals, in Hungarian). In: *Proc. of Present and future of physics in Hungary, Physicist's Meeting, Gödöllõ, Hungary, 25-28 August, 1988,* pp. 214-216. (see also Q.24.)

P.20. E. Beregi, E. Hartmann, L. Malicskó and J. Madarász*: Nd^{3+}, Er^{3+}, ;s Cr^{3+}-mal adalékolt $YAl_3(BO_4)_3$ egykristályok növesztése és morfológiája. (Growth and morphology of $YAl_3(BO_3)_4$ single crystals doped with Nd^{3+}, Er^{3+} és Cr^{3+}, in Hungarian). In: *Proc. of Present and future of physics in Hungary, Physicist's Meeting, Gödöllõ, Hungary, 25-28 August, 1998,* pp. 217-218. (see also Q.21.)

P.21. G. Corradi, K. Polgár, L. Kovács: Újabb perspektívák az ideálist megközelítõ szerkezetû $LiNbO_3$ kristályok kutatásában és alkalmazásában. (New perspectives in the R&D of $LiNbO_3$ crystals with nearly ideal structure, in Hungarian). In: *Proc. of Present and future of physics in Hungary, Physicist's Meeting, Gödöllõ, Hungary, 25-28 August, 1998,* pp. 92-95. (see also Q.22)

P.22. T. Becze-Deák*, L. Bottyán*, G. Corradi, L. Korecz*, D. L. Nagy*, K. Polgár, S. Sayed*, H. Spiering*: A $^{57}Co(EC)^{57}Fe$ elektronbefogást követõen kialakuló töltésállapotok vizsgálata Mg:$LiNbO_3$-ban emissziós Mössbauer-spektroszkópiával. (Investigation of charge states following $^{57}Co(EC)^{57}Fe$ electron capture in Mg:$LiNbO_3$ by Mössbauer emission spectroscopy, in Hungarian). In: *Proc. of Present and future of physics in Hungary, Physicist's Meeting, Gödöllõ, Hungary, 25-28 august, 1998,* pp. 223-225 (see also Q.23.)

Q. CHARACTERIZATION AND POINT DEFECTS OF OPTICAL CRYSTALS

A. Watterich, G. Corradi, E. Hartmann, L. Kovács, L. Malicskó, G. Mandula

Characterization of optical crystals. — The investigation of the morphology of Nd^{3+}, Er^{3+} and Cr^{3+} doped $YAl_3(BO_3)_4$ single crystals showed that the simplest form of a huntite type crystal consists of trigonal prisms and rhombohedra. The YAB:Cr crystals grown by top-seeded solution growth method showed a tabular habit, and were bounded by well developed $\{0001\}$ pinacoid and $\{10\bar{1}1\}$ rhombohedron faces, as well as by small $\{2\bar{2}01\}$ rhombohedra, and a tiny $\{1\bar{1}02\}$ face could also be observed. The prism faces had Miller indices $\{11\bar{2}0\}$ and $\{2\bar{1}\bar{1}0\}$. The other crystals also showed the same forms with varying proportions of the mentioned features.

Microscopy of crystal imperfections. — The application of optical crystals in laser devices requires the knowledge of the structural damage processes induced by irradiations. Using optical and electron microscopic methods we investigated the micromechanisms of structural damage formation caused by different types of optical loadings on absorbing and non-absorbing single crystals such as TeO_2, V_2O_5 and $LiNbO_3$:Fe. It has been found that independent of the laser modes the structural damages in each crystal are initiated by the formation of small voids originating most probably from laser-induced vacancy aggregates.

The as-grown defect structure and composition of Nd^{3+} doped $YAl_3(BO_3)_4$ single crystal has been studied by using optical microscopy and energy dispersive X-ray spectrometry in a scanning electron microscope: compared to the melt composition an excess Al incorporation has been established in the crystal.

Point defects in $ZnWO_4$ and other oxide crystals. — $ZnWO_4$ is used in scintillator detector applications, requiring, however, a better understanding of the luminescence process. Another interesting feature is the low symmetry of the $ZnWO_4$ lattice, making the study of point defects especially rewarding. In Li-doped $ZnWO_4$ (where the presence of Li^+ ions enhances the incorporation of charge compensating OH^- impurity ions) different radiations produce a W^{5+}-type electron center that is perturbed by an OH^- ion. Simultaneously a Li-associated hole-type defect is also produced for charge compensation. In the presence of Mo as an impurity or dopant, similar OH^- ion-perturbed Mo^{5+} defects are created. In Tm-doped crystals the dopant substitutes for Zn^{2+} in the diamagnetic Tm^{3+} state. However, UV-illumination at 77 K creates paramagnetic Tm^{2+} ions, and the observed C_1 symmetry indicates the presence of some local charge compensation. Simultaneously, the illumination also produces Tm-related hole-type defects. All of these centers were characterized and their models were proven by ESR and electron nuclear double resonance (ENDOR) spectroscopy.

Infrared spectroscopy of localized vibrations in oxide crystals. — In sillenite crystals ($Bi_{12}MO_{20}$ with M=Si, Ge, Ti) the localized mode of MO_4 tetrahedra has been studied using infrared absorption spectroscopy. The fundamental and higher harmonics of the asymmetric tetrahedral vibration have been detected in polycrystalline and single crystal samples. The anharmonicity of the mode has been determined using the Morse potential model. Impurities (Im = P, S, V, Mn) occupying tetrahedral sites in sillenites have also been identified by their specific tetrahedral vibration. The presence of additional impurities has modified the stretching mode of

hydroxyl ions and the multi-phonon transitions of both the intrinsic MO_4 and the ImO_4 tetrahedra.

Hydroxyl ions (OH^-) are often present in air-grown crystals. Their stretching vibration has been extensively studied in a number of nonlinear optical crystals (e.g. cesium lithium borate (CLBO), yttrium aluminum borate (YAB), lithium triborate (LBO), and potassium titanyl phosphate (KTP) crystals). Measurements with oriented samples and polarized light were used to determine the direction of the OH^- dipole in the crystal lattice.

Defect structure of $LiNbO_3$. — Progress in the growth of stoichiometric $LiNbO_3$, further increasing its application potential, required the refinement of composition characterization: the method based on the shift of the UV absorption edge was shown to reach a unique value of the relative accuracy (<0.01 mol %) for near stoichiometric compositions. The two-parameter formula found for this calibration greatly simplifies routine characterization.

Ti dopant is used for production of surface waveguides in $LiNbO_3$. Codoping with Mg the Ti ion, normally incorporated on the Li site, was found to substitute for Nb. The ESR signal of this Ti_{Nb}^{3+} center shows an enhanced dynamic Jahn-Teller effect and its vibronic coupling exceeds that of similar centers with d^1 electron structure. Electron transfer from the Ti_{Nb}^{3+} center, resulting in Nb_{Nb}^{4+} polarons, has been stimulated by low temperature illumination in the near UV region. The average energy difference of the involved $Ti^{4+/3+}$ and $Nb^{5+/4+}$ shallow donor states has been estimated to be smaller if the centers occupy Nb sites due to the presence of Mg. This explains the influence of the Mg codopant on refractive index changes and waveguide performance in $LiNbO_3$:Mg crystals treated by Ti in-diffusion.

Photochromic studies have been carried out in pure stoichiometric, congruent and various double-doped congruent $LiNbO_3$ crystals: the effect has been found to be significant only in samples doped with Mg-Fe or Mg-In. Non-resonant microwave absorption detected in double-doped crystals with Mg or Zn as the first and Fe, Cr, or Mn as the second dopant has been explained by the formation of ordered metallic chains.

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Grants

OTKA T 022859	Determination of the structure of point defects by spectroscopic, conductivity and quantum chemical methods. (A. Watterich, 1997-2000)
OTKA T 023092	Characterization of multicomponent nonlinear optical crystals. (E. Hartmann, 1997-2000)
OTKA T 024092	Defect structure studies in $LiNbO_3$ crystals with various compositions and dopants. (G. Corradi, 1997-2000)

OTKA T 026088 Fundamental processes of hologram fixing in photorefractive crystals. (L. Kovács, 1998-2001)

Portuguese-Hungarian Intergovermental S&T Project, P 11/97: Growth and characterization of oxide crystals (G. Corradi 1998-99)

NSF Grant INT-9222297: Point defects in oxide crystals (L.A. Kappers* and A. Watterich, 1994-1998)

Publications

Articles

Q.1. L Malicskó: Structural laser damages in optical crystals. *J. Computer-Assissted Microscopy* **9**, 67-6 8 (1997).

Q.2. A. Watterich, L. A. Kappers* and O. R. Gilliam*: Paramagnetic centers in $ZnWO_4$:Tm single crystals. *Solid State Commun*. **104**, 683-688 (1997).

Q.3. L. Bencs, K. Raksányi, O. Szakács, L.Kovács, A. Watterich and Á. Péter: Removal of iron, chromium and sodium impurities from zinc tungstate ($ZnWO_4$). *J. Crystal Growth*, **181**, 455-458 (1997), (See also P.8.).

Q.4. S. Erdei*, L. Kovács, Á. Petõ*, J. Vandlik*, P. D. Townsend*, F. W. Ainger*: Low temperature three-dimensional thermoluminescence spectra of undoped YVO_4 single crystals grown by different techniques. *J. Appl. Phys.* **82**, 2567-2571 (1997).

Q.5. R. Capelletti*, P. Beneventi*, L. Kovács, A. Ruffini*: FTIR Spectroscopy to Monitor Impurities and Impurity-Interactions in Sillenite Crystals. *Berichte der Bunsen-Gesellschaft für Physikalische Chemie*, **101**, 1282-1285 (1997).

Q.6. A. Watterich and A. Hofstaetter*: O^--Li_{Zn} centers in Li-doped $ZnWO_4$ single crystals characterised by ESR and ENDOR spectroscopy. *Solid State Commun*. **105**, 357-362 (1998).

Q.7. A. Watterich, A. Hofstaetter*, R. Wuerz*, A. Scharmann* and O. R. Gilliam*: Mo^{5+}-H and W^{5+}-H centres in $ZnWO_4$ single crystals characterized by ESR and ENDOR spectroscopy. *J. Phys.: Condensed Matter*, **10,** 205-213 (1998).

Q.8. G. Corradi, I. M. Zaritskii* A. Hofstaetter*, K. Polgár and L. G. Rakitina*: Ti^{3+} on Nb site: A paramagnetic Jahn-Teller center in vacuum-reduced $LiNbO_3$:Mg:Ti single crystals. *Phys. Rev. B* **58**, 8329-37 (1998) (See also P.6.).

Q.9. L. G. Rakitina*, B. D. Shanina*, G. Corradi, K. Polgár: Electron transfer through ordered metallic chains in $LiNbO_3$:(Mg;Zn):Me(3d). *J. Magnetism and Magn. Mater*. **184**, 238-240 (1998). (See also P.4.).

Q.10. E. Beregi, E.Hartmann, L. Malicskó, J. Madarász*: Growth and morphology of Nd^{3+}, Er^{3+} and Cr^{3+} doped $YAl_3(BO_3)_4$ single crystals. *Crystal Research and Technology*, accepted for publication (See also P.14.).

Q.11. L. A. Kappers*, O. R. Gilliam*, R. H. Bartram*, I. Földvári, A. Watterich: A study of optical and ESR radiation-induced absorptions in TeO_2 single crystals.

Radiation Effects and Defects in Solids, accepted for publication (See also P.12.).

Q.12. A. Watterich, L. A. Kappers*, O. R. Gilliam*: Sn-related paramagnetic defects in UV-illuminated $ZnWO_4$ single crystals. *J. Phys.: Condensed Matter*, accepted for publication.

Q.13. P. Beneventi*, B. Briat*, R. Capelletti*, M. Gospodinov*, L. Kovács, E. Mazocchi*, A. Ruffini*: Electronic and vibrational levels of the photochromic Mn in sillenites. *Radiation Effects and Defects in Solids*, accepted for publication.

Q.14. G. Corradi, L. Kovács and I. M. Zaritskii*: Optical absorption edge and some shallow donor levels in $LiNbO_3$ systems. *Radiation Effects and Defects in Solids*, accepted for publication.

Q.15. L. Grigorjeva*, D. Millers*, G. Corradi, K. Polgár and V. Pankratov*: Induced optical absorption and relaxation process in $LiNbO_3$. *Radiation Effects and Defects in Solids*, accepted for publication (See also P.16.).

Conference proceedings

Q.16. A. Watterich, L. Kovács, E. Hartmann, M.T. Borowiec*, B. Briat*: Complex study of photo-induced defects in V-doped $Bi_4Ge_3O_{12}$. In: *Proceedings of International Conference on Solid State Crystals, Zakopane, Poland, 12-16 Oct. 1998.*, SPIE, accepted for publication.

Q.17. L. Kovács, E. Beregi, K. Polgár, Á. Péter: FTIR spectroscopy of borate crystals. In: *Proceedings of International Conference on Solid State Crystals, 12-16 Oct. 1998, Zakopane, Poland,* SPIE, accepted for publication (See also P.17.).

Q.18. M. T. Borowiec*, H. Szymczak*, M. Zaleski*, P. Kaczor*, L. Adamowicz*, J. Strzeszewski*, A. Watterich, L. Kovács: Raman and IR spectroscopy investigations of double tungstates. In: *Proceedings of International Conference on Solid State Crystals, 12-16 Oct. 1998, Zakopane, Poland,* SPIE, accepted for publication.

Book chapters

Q.19. J. Giber*, E. Hartmann: Diffúzió ionkristályokban. Ionos vezetés. (Diffusion in ionic crystals. Ionic conductivity, in Hungarian). In: *Diffúzió és implantáció szilárdtestekben* (*Diffusion and implantation in solids),* Eds.: J. Giber, J. Gyulai, Mûegyetemi Kiadó, Budapest 1997, pp. 211-255.

Q.20. E. Hartmann: Gyulai Zoltán. In: *Magyar Tudóslexikon A-tól Z-ig* (*Biographies of Hungarian scientists A-Z,* in Hungarian*),* Ed. Ferenc Nagy, Better-MTESZ-OMIKK, Budapest 1997. pp. 353-355.

Others

Q.21. E. Beregi, E. Hartmann, L. Malicskó, J. Madarász*: Nd^{3+}, Er^{3+} és Cr^{3+} -mal adalékolt $YAl_3(BO_3)_4$ egykristályok növesztése és morfológiája (Growth and

morphology of Nd^{3+}, Er^{3+} and Cr^{3+} doped $YAl_3(BO_3)_4$ single crystals, in Hungarian). In: *Present and future of physics in Hungary, Physicist's Meeting, Gödöllõ, 25-28 August, Gödöllõ, Hungary, 1998.* pp. 217-218. (See also P.20.).

Q.22. G. Corradi, K. Polgár, L. Kovács: Újabb perspektívák az ideálist megközelítõ szerkezetû $LiNbO_3$ kristályok kutatásában és alkalmazásában (New perspectives in the R&D of $LiNbO_3$ crystals with nearly ideal structure, in Hungarian). In: *Present and future of physics in Hungary, Physicist's Meeting, Gödöllõ, 25-28 august, 1998*, pp. 92-95 (See also P.21.).

Q.23. T. Becze-Deák*, L. Bottyán*, G. Corradi, L. Korecz*, D. L. Nagy*, K. Polgár, S. Sayed*, H. Spiering*: A $^{57}Co(EC)^{57}Fe$ elektronbefogást követõen kialakuló töltésállapotok vizsgálata Mg:$LiNbO_3$-ban emissziós Mössbauer-spektroszkópiával (Investigation of charge states following $^{57}Co(EC)^{57}Fe$ electron capture in Mg:$LiNbO_3$ by Mössbauer emission spectroscopy, in Hungarian). In: *Present and future of physics in Hungary, Physicist's Meeting, Gödöllõ, 25-28 august, 1998*, pp. 223-225 (See also P.22.)

Q.24. Beregi E., Izvekov V.*, Kovács L., Péter Á., Polgár K.: FTIR spektroszkópiai vizsgálatok borát kristályokon (FTIR spectroscopical studies on borate crystals, in Hungarian). In: *Present and future of physics in Hungary, Physicist's Meeting)* Gödöllõ, 25-28 August, 1998, pp. 214-216. (See also P.19.).

Q.25. L. Malicskó : Réteges kristálynövekedés és következményei. (Layer-by-layer growth of crystals and its consequences, in Hungarian). In: *Present and future of physics in Hungary, Physicist's Meeting, Gödöllõ, 25-28 August, 1998*, pp. 219-220.

Q.26. G. Mandula: Fotovezetés és fotorefrakció kettõsen adalékolt $LiNbO_3$ kristályokban. (Photoconductivity and photorefraction in doubly-doped $LiNbO_3$ crystals, in Hungarian). *Present and future of physics in Hungary, Physicist's Meeting, Gödöllõ, 25-28 August, 1998*, pp. 221-222.

Q.27. L. Malicskó: Folyamat-indukálta kristályhibák oxidkristályokban.(Process-induced crystal defects in optical oxide crystals). *Special Transactions of the University of Veszprém.* Ed. by K. Kovács. Invited review paper, accepted for publication.

R. NONLINEAR AND QUANTUM OPTICS

P. Ádám, P. Domokos, J. Janszky, Zs. Kis, T. Kiss, Sz. Szabó, V. Szalay

Quantum state reconstruction. — We continued our studies on methods to reconstruct the quantum mechanical state of nonclassical light fields. We proposed a new scheme combining unbalanced and balanced homodyne detection. This scheme has the advantage that quasiprobability distributions in phase space are scanned point-by-point, adjusted by the first local oscillator. We have calculated the analytic form of the corresponding local sampling function. Our numerical simulations suggest the feasibility of the method.

Cavity quantum electrodynamics. — We showed that the use of a single atom allows one to prepare an arbitrary photon number state (Fock state) in a high Q cavity. The atom undergoes a controlled succession of interactions with two cavity modes. One of them contains a classical coherent field from which the atom transfers photons, one by one, to the initially empty second mode. The scheme can be extended to prepare a quantum superposition of the vacuum state with a Fock state, a highly non-classical field. The feasibility of the proposed experiment has been verified for the case of a microwave cavity interacting with circular Rydberg atoms. We showed, by means of numerical simulation, that almost perfect three photon state can be generated at the present state of art in experimental cavity QED.

We participated in the realization of a neodymium-doped silica microsphere laser, of diameters in the range of 50-100 μm. Following very low threshold observed at room temperature (absorbed pump power of 200 nW), we aimed to operate the laser in a cryogenic setup at 2K. Very high Q quality factor, $Q = 3 \cdot 10^8$, has been preserved for the whispering gallery modes of a 50 μm diameter microsphere immersed in a superfluid Helium. The homogenous linewidth of the active medium is radically reduced at this temperature. Preliminary results on lasing at this temperature have also been obtained as a first step toward a “thresholdless laser” regime. The quantum theory of microlasers operating in the strong coupling regime has been developed to give an account for the anticipated thresholdless behaviour.

Nonclassical field states —A coherent-state representation of the Hilbert-space of the harmonic oscillator is developed. The basis set consists of the coherent states with real parameter which are in an infinitesimal vicinity of zero. Properties of star states generated in a three-photon down-conversion process are analyzed. It is shown, that the absorption efficiency of these states in three-photon processes is orders of magnitude larger than that of the coherent light.

Nuclear motions in molecules. — We have developed continuos contracted distributed approximating functions for Feynman path integration in real time. We have shown how contracted Hermite distributed approximating functions can be employed in solving vibrational eigenvalue problems. We have given a solution to a more than 40 year old puzzle, the derivation of internal axis system of molecules with asymmetric top and asymmetric frame, in theoretical molecular spectroscopy.

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Grants:

OTKA T 017386	Nonlinear optical processes and nonclassical states (P. Adam, 1995-1998).
OTKA F 017380	Quantum electrodynamics in cavities (P. Domokos, 1995-1998)
OTKA F 017381	Squeezed states in Paul-traps (T. Kiss, 1995-1998)
OTKA F 019232	Quantum optical processes in oscillator systems (Zs. Kis, 1996-1999)
OTKA T 023777	Effects of nonclassical states of light on atom optical phenomena (J. Janszky, 1997-2000)
OTKA F 023617	Phase squeezed and phase optimized quantum states of light (Sz. Szabó, 1997-2000)
OTKA T 025103	Vibrational potentional energy surfaces of molecules, the direct and the inverse spectroscopic problems (V. Szalay, 1998-2000)

Publications:

Articles

R.1. P. Domokos, M. Brune*, J. M. Raimond* and S. Haroche*: Photon-number state generation with a single two-level atom in a cavity, a proposal. *European Phys. Journal* **1**, 1-4 (1998).

R.2. F. Treussart*, V. S. Ilchenko*, J. F. Roch*, P. Domokos, J. Hare*, V. Lefevre*, J. M. Raimond* and S. Haroche*: Whispering gallery mode microlaser at liquid He temperature. *Journal of Luminescence* **77**, 670-673 (1998).

R.3. S. Szabó, P. Domokos, P. Ádám, and J. Janszky: Coherent-state representation of an infinitesimal interval in phase space. *Phys. Lett.* A **241**, 203-206 (1998).

R.4. J. Janszky, Z. Kis, and P. Ádám: Star states. *Forschr. Phys.* **46**, 6-8 (1998).

R.5. V. Szalay, Contracted distributed approximating functions: Derivation of non-oscillatory free particle and harmonic propagators for Feynman path integration in real time. *J. Chem. Phys.* **108**, 2847-2866 (1998).

R.5. V. Szalay and J. Ortigoso*: The internal axis system of molecules with one large amplitude internal motion. *J. Chem. Phys.* **109**, 3911-3918 (1998).

R.6. T. Kiss, U. Herzog* and U. Leonhardt*: Reply to 'Loss-error compensation im quantum-state measurements'. *Phys. Rev.* **A57,** 3134-3135 (1998)

R.7. Z. Kis, T. Kiss, J. Janszky, P. Ádám, S. Wallentowitz*, and W. Vogel*: Local sampling of phase-space distribution by cascaded optical homodyning. *Phys. Rev. A* , accepted for publication.

R.8. U. Leonhardt*, T. Kiss, and P. J. Bardoff*: State reconstruction of wave packets moving in time-dependent potentials and the existence of Wronskian pairs. *J. Phys. A* , accepted for publication.

R.9. V. Szalay and S. C. Smith*: Application of contracted distributed approximating functions to solving vibrational eigenvalue problems. *J. Chem. Phys*., accepted for publication.

R.10. I. Protsenko*, P. Domokos, V. Lefevre*, J. Hare*, J. M. Raimond*, and L. Davidovich*: Quantum theory of a thresholdless laser. *Phys. Rev. A*, accepted for publication.

Conference proceedings

R.11. P. Ádám, T. Kiss, and J. Janszky: Planning the evolution of time-dependent oscillators. In: *Proc. of the Fifth International Conference on Squeezed States and Uncertanity Relations, Balatonfüred, Hungary*, 1997, Eds. D. Han, J. Janszky, Y. S. Kim, V.I. Man'ko, NASA/CP-1998-206855, 1998, pp. 189-194.

R.12. P. Ádám, J. Janszky, S. Szabó, E. Lugosi*: Relations between input and output states of integrated optical systems. In: *Proc. of 5th Congress on Modern Optics, Optika'98, Budapest, Hungary*, Eds. Gy. Akos, G. Lupkovics, and A. Podmaniczky, Proc. of SPIE vol. 3573, 1998, pp. 55-58.

R.13. Z. Kis, J. Janszky, P. Ádám: Star states in multiphoton processes. In: *Proc. of 5th Congress on Modern Optics, Optika'98, Budapest, Hungary*, Eds. Gy. Akos, G. Lupkovics, and A. Podmaniczky, Proc. of SPIE vol. 3573, 1998, pp. 74-77.

Book

R.14. Császár Attila* és Szalay Viktor: Molekularezgések elméleti vizsgálata. A Kémia Újabb Eredményei. (Theoretical study of molecular vibrations, Progress in Chemistry), Akadémiai Kiadó, 1998.

Other

R.15. V. Szalay and S. C. Smith*: Application of contracted distributed approximating functions to solving vibrational eigenvalue problems. P057 *Book of Abstracts of The 2nd Australian Conference on Physical Chemistry, University of Brisbane, Brisbane, 11-15 July 1998*.

EDUCATION

Graduate and postgraduate courses, 1998

- Theory of Magnetism I. (P. Fazekas, BME[3])
- Theory of Magnetism II. (P. Fazekas, BME)
- Statistical physics (F. Iglói, JATE[4])
- Thermodynamics and statistical physics (F. Iglói, JATE)
- Advanced Solid state physics I. (J. Sólyom, ELTE[5])
- Advanced Solid State Physics II. (J. Sólyom, ELTE)
- Advanced Solid State Physics III. (I. Tüttõ, ELTE)
- Superconductivity (I. Tüttõ, BME)
- Broken symmetry states in condensed matter (I. Tüttõ, ELTE)
- Completely integrable many body systems (F. Woynarovich, ELTE-BME)
- Electrodynamics II. (F. Woynarovich, ELTE)
- Solid state physics II. (A. Virosztek, BME)
- Solid state physics III. (A. Virosztek, BME)
- Electronic Structure of Solids (J. Kollár, ELTE)
- Solid state research I. (I. Vincze, ELTE)
- Amorphous and crystalline materials (P. Deák*, S. Kugler* and T.Kemény, BME)
- Structure and Properties of Non-Equilibrium Alloys (T. Kemény, ELTE)
- Nucleation theory (L. Gránásy, ELTE)
- Macromolecules (S. Pekker, ELTE)
- Spectroscopy and materials structure (K. Kamarás, BME)
- Group theory in solid state research (K.Kamarás, BME)
- Methods in materials science (K.Kamarás BME)
- Solid State Physics I. (G. Kriza, BME)
- Synthesis of Liquid Crystals (K.Fodor-Csorba, ELTE)
- Physics of liquid crystals and polymers (Á. Buka, ELTE)
- Pattern formation in complex systems (Á. Buka, ELTE)
- Nanophase metals: electrical transport and magnetic properties (I. Bakonyi, ELTE)
- Advanced material technology (G. Konczos, BME)

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[5] ELTE: Loránd Eötvös University, Budapest

- NMR spectroscopy (K. Tompa, BME)
- Neutron Scattering (L. Cser, ELTE)
- Neutron Scattering in Condensed Matter (L. Rosta, BME)
- Materials Testing with Neutrons (L. Cser, BME)
- Optical methods in solid state physics (Zs. Szentirmay, ELTE)
- Physics of Optical Crystals (I. Földvári, Á. Péter, BME)
- Crystal Growth from the Melt (in: Crystalline and Amorphous Materials, K. Polgár, BME)
- Physics of dielectrics (E. Hartmann, A. Tóth*, BME)
- Theories of crystal growth (L.Malicskó, BME)
- Oxide crystals for non-linear optical applications (L. Kovács, University of Parma)
- Statistical quantum optics I-II. (J. Janszky, P. Ádám, ELTE)
- Quantum optics I. (J. Janszky, P. Ádám, Z. Kis, JATE)
- Experimental quantum optics (J. Janszky, P. Ádám, Z. Kis, JATE)
- Quantum mechanics I. (P.Ádám, JPTE[6])
- Quantum mechanics II. (P. Ádám, JPTE)
- Nonclassical light (P. Ádám, JPTE)
- Atom traps (P. Ádám, JPTE)

Laboratory practice and seminars

- Thermodynamics and statistical physics seminar (A. Rákos, ELTE)
- Solid state physics seminar (J. Sólyom, ELTE)
- Laboratory for solid state physics, Preparation and crystallization of metallic glasses (I. Vincze, ELTE)
- Basic experimental physics (L. Gránásy, A Jákli, BME)
- Atomic and molecular physics laboratory, (K. Kamarás, ELTE)
- Solid State Physics Seminar (G. Kriza, BME)
- Advanced Solid State Physics Laboratory (I. Pethes, BME, ELTE)
- Experiments on liquid crystals (Á. Buka, ELTE)
- NMR spectroscopy (K. Tompa, ELTE)
- Engineering materials and technology I., II., III. (J. Garaguly, BME)
- Programming practice (I. Varga, BME)
- Metallography (B. Varga, BME)

[6] JPTE: Janus Pannonius University, Pécs

- Welding (B. Varga, BME)
- Neutron Scattering (L. Rosta, S. Borbély, BME)
- Experimental Methods in Neutron Physics (L. Rosta, S. Borbély, BME)
- Modern optical laboratory (Gain and mode structure of gas lasers) (G. Bánó, BME)
- Medical application of lasers (Z. Gy. Horváth ; HIETE[7], Medical Laser Center)
- Measurements on an experimental He-Ne laser (K. Szőcs, BME)
- Seminars on biophysics for medical students (K. Szőcs, SOTE[8])
- General physics, seminar (Sz. Fórizs, BME)
- Seminars on laser optics (Zs. Szentirmay, ELTE)
- Laser optical laboratory (Zs. Szentirmay, ELTE)
- Hologram recording in oxide crystals (L. Kovács and G. Mandula, ELTE)
- Quantum mechanics, (Z. Kis, JPTE)
- Theoretical physics seminar (P. Ádám, JPTE)

Diploma works

- P. Varga (BME): Inverse lifetime and Hall-effect in high temperature superconductors (Consultant: A. Virosztek)
- J. Fortágh (BME): A linear microtrap for neutral atoms (Consultant: A. Virosztek)
- Z. Váradi (BME): Influence of smectic fluctuations on electrohydrodynamic instabilities of the nematic liquid crystal phase (Consultant: Á. Buka)
- S. Ungi (BME): Study of phase relationships in rapidly quenched iron-based dilute alloys (Consultant: A. Lovas)
- E. Rétfalvi (BME): Neutron scattering study of structural metals of technological importance (Consultant: L.Rosta)
- K. Kutasi (Babes-Bólyai University, Cluj, Romania): Gain measurements on He-Cu lasers in segmented hollow cathode discharges (Consultant: Z. Donkó)

Ph. D. students

I. Pethes: Experiments on moving glasses (Supervisor: G. Kriza)

T. Tóth Katona: Pattern formation at the interfaces of liquid crystal phases (Supervisor: Á. Buka)

T. Börzsönyi: Oscillatory shear induced instabilities in nematic liquid crystals (Supervisor: Á. Buka)

[7] HIETE: Imre Hajnal Medical University, Budapest

[8] SOTE: Semmelweis Medical University, Budapest

D. Goldschmidt: Interferometric studies of patterns in liquid crystals (Supervisor: Á. Buka)

M. Bokor (ELTE): NMR relaxation in Fe and Zn ionic crystals (Supervisor: K. Tompa)

A. Kákay (ELTE): Magnetic nanocomposites: modelling and experiments (Supervisor: L.K. Varga)

T. Marek (ELTE): NMR spectra in Fe and Zn ionic crystals (Supervisor: K. Tompa)

B. Varga (BME): Study of phase transformations in rapidly quenched micro- and nanocrystalline alloys by magnetic measurements (Supervisor: A. Lovas)

I. Varga (BME): Magnetic domain contrast studies and image processing by SEM (Supervisor: L. Pogány)

L. Almásy: Investigation of metastable sytems by neutron scattering (Supervisor: L. Cser)

P. Jóvári: Structure investigation of solutions using neutron scattering and quantum chemical approaches. (Supervisor: L. Cser)

E. Rétfalvi: Irradiation damage study of materials of technological importance by neutron scattering technique (Supervisor: L. Rosta)

L. Szalai (JATE): Au laser in segmented hollow cathode discharge (Supervisors: K. Rózsa and Z. Donkó)

G. Bánó (JATE): Cathode sputtered Zn laser (Supervisors: K. Rózsa and Z. Donkó)

K. Szõcs (SOTE): Fluorescence imaging (Supervisor: Z. Gy. Horváth)

Sz. Fórizs (BME): Application of neurochips in optics (Supervisor: Z. Gy. Horváth)

F. Lhommé (Université de Metz): Study of the intrinsic and extrinsic defects in lithium niobat doped with chrome (Hungarian co-leader: K. Polgár)

P. Ney (Université de Metz): Study of the electro-optical and nonlinear optical properties of β-barium metaborate by Raman-spectroscopy (Hungarian co-adviser: K. Polgár)

J. Almgren: Growth and structure of rubidium titanyl arsenat and related compounds (Chalmers University, Göteborg, Hungarian co-adviser: Á. Péter)

P. Domokos: Cavity quantum electrodynamics (Supervisor: J. Janszky)

T. Kiss: Methods to reconstruct the quantum states of light (Supervisor: J. Janszky)

Z. Kis: Nonclassical vibrational states (Supervisor: J. Janszky)

S. Szabó: Low dimensional coherent state representations of the quantum states of light (Supervisor: J. Janszky)

Dissertations

Ö. Legeza: One dimensional and coupled spin chains with the density matrix renormalization method (Ph.D., BME)

G. Faigel: Nuclear scattering in solid state physics (Doctor of Physical Science, Hungarian Academy of Sciences)

T. Tóth Katona: Pattern forming instabilities of the nematic – smectic B interface (Ph. D., ELTE TTK)

J. Garaguly: Study of hydrogen absorption-desorption processes in amorphous alloys by in-situ resistivity measurements (Ph.D., BME)

Á. Hofmann: Investigation of noble metal thin films using the method of the attenuated total reflection (Ph.D., BME)

AWARDS

P. Fazekas, Széchenyi Grant (1998-2001)

F. Iglói, Széchenyi Grant (1997-2001)

B. Újfalussy, Award for young Scientists of the Hungarian Academy of Sciences

Á. Buka, Széchenyi Grant (1997-2001)

G. Oszlányi, Bólyai Grant (1998-2001)

T. Pusztai, Soros Grant (1998-2001)

Z. Donkó, R. Schmid Award of the Eötvös Physical Sociaty

Z. Donkó, Bólyai Grant (1998-2001)

E. Hartmann, Gyulai Award, Roland Eötvös Physical Society, Budapest.

J. Janszky, Széchenyi Grant (1998-2001)

P. Ádám, Széchenyi Grant (1997-2000)

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